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PositiveIntegrators.jl: A Julia library of positivity-preserving time integration methods

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Summary

We introduce PositiveIntegrators.jl, a Julia package that provides efficient implementations of various time integration schemes for the solution of positive ordinary differential equations, making these methods accessible for users and comparable for researchers. Currently, the package provides the unconditionally positivity-preserving MPRK, SSP-MPRK, and MPDeC schemes, which are also conservative when applied to a conservative system. The package is fully compatible with DifferentialEquations.jl, which allows a direct comparison between the provided schemes and standard methods.

Statement of need

Many systems of ordinary differential equations that model real-life applications have positive solutions. For some of these systems unconditionally positivity-preserving time integration methods are helpful or even necessary to obtain meaningful solutions.

Unfortunately, positivity is not preserved in almost any of the standard time integration schemes, such as Runge–Kutta methods, Rosenbrock methods, or linear multistep methods. In particular, higher-order general linear methods cannot preserve positivity unconditionally (Bolley & Crouzeix, 1978). The only standard scheme with which unconditional positivity can be achieved is the implicit Euler method (assuming that the nonlinear systems are solved exactly). However, this is only first-order accurate and the preservation of positivity within the nonlinear iteration process poses a problem. For example, it may happen that the right-hand side of the differential equation is only defined for nonnegative values and would throw an error if a negative value is passed to it, e.g., in the case of a square root. Standard nonlinear solvers like Newton's method or fixed-point iterations will in general not only produce iterates that are nonnegative, causing the iteration to fail. Another strategy for preserving positivity used in existing open source or commercial packages (like MATLAB) is to set negative solution components that are accepted by the step size control to zero. Unfortunately, this can have a negative impact on possible conservation properties. Further approaches in the literature include projections in between time steps (Nüßlein et al., 2021; Sandu, 2001), if a negative solution was computed, or it is tried to reduce the time step size as long as a nonnegative solution is calculated. Finally, strong stability preserving (SSP) methods can also be used to preserve positivity, but this is again subject to step size limitations (Gottlieb et al., 2011).

Consequently, various new, unconditionally positive schemes have been introduced in recent years, see Burchard et al. (2003), Bruggeman et al. (2007), Broekhuizen et al. (2008), Formaggia & Scotti (2011), Ortleb & Hundsdorfer (2017), Kopecz & Meister (2018a), Kopecz & Meister (2018b), Huang & Shu (2019), Huang et al. (2019), Öffner & Torlo (2020), Martiradonna et al. (2020), Ávila et al. (2020), Ávila et al. (2021), Blanes et al. (2022), Zhu et al. (2024), Izzo et al. (2025), and Izgin et al. (2025). Among these, most of the literature

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is devoted to modified Patankar–Runge–Kutta (MPRK) methods.

Unfortunately, these new methods are not yet available in software packages, making them inaccessible to most users and limiting their comparability within the scientific community. PositiveIntegrators.jl aims at making these methods available and thus usable and comparable.

Features

PositiveIntegrators.jl is written in Julia (Bezanson et al., 2017) and makes use of its strengths for scientific computing, e.g., ease of use and performance. The package is fully compatible with DifferentialEquations.jl (Rackauckas & Nie, 2017) and therefore many features that are available there can be used directly. In particular, this allows a direct comparison of the provided methods and standard schemes. Moreover, it integrates well with the Julia ecosystem, e.g., by making it simple to visualize numerical solutions using dense output in Plots.jl (Christ et al., 2023).

The package offers implementations of conservative as well as non-conservative production-destruction systems (PDS), which are the building blocks for the solution of differential equations with MPRK schemes. Furthermore, conversions of these PDS to standard `ODEProblems` from DifferentialEquations.jl are provided.

Currently, the package contains the following methods:

- The MPRK methods `MPE`, `MPRK22`, `MPRK43I`, and `MPRK43II` of Kopecz & Meister (2018a) and Kopecz & Meister (2018b) are based on the classical formulation of Runge–Kutta schemes and have accuracies from first to third order.
- The MPRK methods `SSPMPRK22` and `SSPMPRK43` of Huang & Shu (2019) and Huang et al. (2019) are based on the SSP formulation of Runge–Kutta schemes and are of second and third order, respectively.
- The `MPDeC` methods of Öffner & Torlo (2020) combine the deferred correction approach with the idea of MPRK schemes to obtain schemes of arbitrary order. In the package methods from second up to 10th order are implemented.

In addition, all implemented methods have been extended so that non-conservative and non-autonomous PDS can be solved as well. Furthermore, adaptive step size control is available for almost all schemes.

Related research and software

The first MPRK methods were introduced by Burchard et al. (2003). These are the first-order scheme `MPE` and a second-order scheme based on Heun's method. To avoid the restriction to Heun's method, the second-order `MPRK22` schemes were developed by Kopecz & Meister (2018a). The techniques developed therein also enabled a generalization to third-order schemes and thus the introduction of `MPRK43I` and `MPRK43II` methods by Kopecz & Meister (2018b).

The aforementioned schemes were derived from the classical formulation of Runge-Kutta methods. Using the Shu-Osher formulation instead lead to the introduction of the second-order schemes `SSPMPRK22` by Huang & Shu (2019) and the third-order scheme `SSPMPRK43` by Huang et al. (2019).

Starting from a low-order method, the deferred correction approach can be used to increase the method's approximation order iteratively. Öffner & Torlo (2020) combined deferred correction with the MPRK idea to devise MPRK schemes of arbitrary order. These are implemented as `MPDeC` schemes for orders 2 up to 10.

The implemented methods were originally introduced for conservative production-destruction systems only. An extension to non-conservative production-destruction systems was presented by Meister & Benz (2015). We implemented a modification of this algorithm, by treating the non-conservative production and destruction terms separately, weighting the destruction terms and leaving the production terms unweighted.

Readers interested in additional theoretical background, further properties of the implemented schemes, and some applications are referred to the publications of Kopecz & Meister (2019), Izgin et al. (2022a), Izgin et al. (2022b), Huang et al. (2023), Torlo et al. (2022), and Izgin & Öffner (2023). PositiveIntegrators.jl was successfully applied in the work of Bartel et al. (2024) to solve Fokker-Planck equations, ensuring the positivity of the unknown quantities.

Existing software libraries do not have a strong focus on unconditional positivity and, to the authors' knowledge, there is no other software library offering MPRK schemes. A common strategy to obtain nonnegative solutions used in the `PositiveDomain` callback of DifferentialEquations.jl or the commercial package MATLAB is described by Shampine et al. (2005). In this approach negative components of approximate solutions that have been accepted by the adaptive time stepping algorithm are set to zero. Another possibility is to reduce the chosen time step size beyond accuracy considerations until a nonnegative approximation is calculated. This can be achieved in DifferentialEquations.jl using the solver option `isoutofdomain`.

We also mention that some papers on MPRK schemes offer supplementary codes. However, these are mainly small scripts for the reproduction of results shown in the papers and are not intended as software libraries.

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References

Ávila, A. I., González, G. J., Kopecz, S., & Meister, A. (2021). Extension of modified Patankar-Runge-Kutta schemes to nonautonomous production-destruction systems based on Oliver's approach. *Journal of Computational and Applied Mathematics*, *389*, Paper No. 113350, 13. https://doi.org/10.1016/j.cam.2020.113350

Ávila, A. I., Kopecz, S., & Meister, A. (2020). A comprehensive theory on generalized BBKS schemes. *Applied Numerical Mathematics*, *157*, 19–37. https://doi.org/10.1016/j.apnum.2020.05.027

Bartel, H., Lampert, J., & Ranocha, H. (2024). Structure-preserving numerical methods for Fokker-Planck equations. *Proceedings in Applied Mathematics and Mechanics*, e202400007. https://doi.org/10.1002/pamm.202400007

Bezanson, J., Edelman, A., Karpinski, S., & Shah, V. B. (2017). Julia: A fresh approach to numerical computing. *SIAM Review*, *59*(1), 65–98. https://doi.org/10.1137/141000671

Blanes, S., Iserles, A., & Macnamara, S. (2022). Positivity-preserving methods for ordinary differential equations. *ESAIM. Mathematical Modelling and Numerical Analysis*, *56*(6), 1843–1870. https://doi.org/10.1051/m2an/2022042

Bolley, C., & Crouzeix, M. (1978). Conservation de la positivité lors de la discrétisation des problèmes d'évolution paraboliques. *RAIRO. Analyse Numérique*, *12*(3), 237–245. https://doi.org/10.1051/m2an/1978120302371

Broekhuizen, N., Rickard, G. J., Bruggeman, J., & Meister, A. (2008). An improved and generalized second order, unconditionally positive, mass conserving integration scheme for biochemical systems. *Applied Numerical Mathematics*, *58*(3), 319–340. https://doi.org/10.1016/j.apnum.2006.12.002

Bruggeman, J., Burchard, H., Kooi, B. W., & Sommeijer, B. (2007). A second-order, unconditionally positive, mass-conserving integration scheme for biochemical systems. *Applied Numerical Mathematics*, *57*(1), 36–58. https://doi.org/10.1016/j.apnum.2005.12.001

Burchard, H., Deleersnijder, E., & Meister, A. (2003). A high-order conservative Patankar-type discretisation for stiff systems of production–destruction equations. *Applied Numerical Mathematics*, *47*(1), 1–30. https://doi.org/10.1016/S0168-9274(03)00101-6

Christ, S., Schwabeneder, D., Rackauckas, C., Borregaard, M. K., & Breloff, T. (2023). Plots.jl — a user extendable plotting API for the Julia programming language. *Journal of Open Research Software*, *11*(1), 5. https://doi.org/10.5334/jors.431

Formaggia, L., & Scotti, A. (2011). Positivity and conservation properties of some integration schemes for mass action kinetics. *SIAM Journal on Numerical Analysis*, *49*(3), 1267–1288. https://doi.org/10.1137/100789592

Gottlieb, S., Ketcheson, D. I., & Shu, C.-W. (2011). *Strong stability preserving Runge-Kutta and multistep time discretizations*. World Scientific. https://doi.org/10.1142/7498

Huang, J., Izgin, T., Kopecz, S., Meister, A., & Shu, C.-W. (2023). On the stability of strong-stability-preserving modified Patankar-Runge-Kutta schemes. *ESAIM: Mathematical Modelling and Numerical Analysis*, *57*(2), 1063–1086. https://doi.org/10.1051/m2an/2023005

Huang, J., & Shu, C.-W. (2019). Positivity-preserving time discretizations for production-destruction equations with applications to non-equilibrium flows. *Journal of Scientific Computing*, *78*(3), 1811–1839. https://doi.org/10.1007/s10915-018-0852-1

Huang, J., Zhao, W., & Shu, C.-W. (2019). A third-order unconditionally positivity-preserving scheme for production-destruction equations with applications to non-equilibrium flows. *Journal of Scientific Computing*, *79*(2), 1015–1056. https://doi.org/10.1007/s10915-018-0881-9

Izgin, T., Ketcheson, D. I., & Meister, A. (2025). Order conditions for Runge–Kutta-like methods with solution-dependent coefficients. *Communications in Applied Mathematics and Computational Science*, *20*(1), 29–66. https://doi.org/10.2140/camcos.2025.20.29

Izgin, T., Kopecz, S., & Meister, A. (2022a). On Lyapunov stability of positive and conservative time integrators and application to second order modified Patankar-Runge-Kutta schemes. *ESAIM: Mathematical Modelling and Numerical Analysis*, *56*(3), 1053–1080. https://doi.org/10.1051/m2an/2022031

Izgin, T., Kopecz, S., & Meister, A. (2022b). On the stability of unconditionally positive and linear invariants preserving time integration schemes. *SIAM Journal on Numerical Analysis*, *60*(6), 3029–3051. https://doi.org/10.1137/22M1480318

Izgin, T., & Öffner, P. (2023). A study of the local dynamics of modified Patankar DeC and higher order modified Patankar-RK methods. *ESAIM: Mathematical Modelling and Numerical Analysis*, *57*(4), 2319–2348. https://doi.org/10.1051/m2an/2023053

Izzo, G., Messina, E., Pezzella, M., & Vecchio, A. (2025). Modified Patankar linear multistep methods for production-destruction systems. *Journal of Scientific Computing*, *102*(3), Paper No. 87, 39. https://doi.org/10.1007/s10915-025-02804-5

Kopecz, S., & Meister, A. (2018a). On order conditions for modified Patankar-Runge-Kutta schemes. *Applied Numerical Mathematics*, *123*, 159–179. https://doi.org/10.1016/j.

apnum.2017.09.004

Kopecz, S., & Meister, A. (2018b). Unconditionally positive and conservative third order modified Patankar-Runge-Kutta discretizations of production–destruction systems. *BIT Numerical Mathematics*, *58*(3), 691–728. https://doi.org/10.1007/s10543-018-0705-1

Kopecz, S., & Meister, A. (2019). On the existence of three-stage third-order modified Patankar-Runge-Kutta schemes. *Numerical Algorithms*, 1–12. https://doi.org/10.1007/s11075-019-00680-3

Martiradonna, A., Colonna, G., & Diele, F. (2020). *GeCo*: Geometric Conservative nonstandard schemes for biochemical systems. *Applied Numerical Mathematics*, *155*, 38–57. https://doi.org/10.1016/j.apnum.2019.12.004

Meister, A., & Benz, J. (2015). Phosphorus cycles in lakes and rivers: Modeling, analysis, and simulation. In W. Freeden, M. Z. Nashed, & T. Sonar (Eds.), *Handbook of geomathematics* (pp. 1387–1416). Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-642-54551-1_23

Nüßlein, S., Ranocha, H., & Ketcheson, D. I. (2021). Positivity-preserving adaptive Runge-Kutta methods. *Communications in Applied Mathematics and Computational Science*, *16*(2), 155–179. https://doi.org/10.2140/camcos.2021.16.155

Öffner, P., & Torlo, D. (2020). Arbitrary high-order, conservative and positivity preserving Patankar-type deferred correction schemes. *Applied Numerical Mathematics*, *153*, 15–34. https://doi.org/10.1016/j.apnum.2020.01.025

Ortleb, S., & Hundsdorfer, W. (2017). Patankar-type runge-kutta schemes for linear PDEs. *AIP Conference Proceedings*, *1863*(1), 320008. https://doi.org/10.1063/1.4992489

Rackauckas, C., & Nie, Q. (2017). DifferentialEquations.jl – A performant and feature-rich ecosystem for solving differential equations in Julia. *Journal of Open Research Software*, *5*(1), 15. https://doi.org/10.5334/jors.151

Sandu, A. (2001). Positive numerical integration methods for chemical kinetic systems. *Journal of Computational Physics*, *170*(2), 589–602. https://doi.org/10.1006/jcph.2001.6750

Shampine, L. F., Thompson, S., Kierzenka, J. A., & Byrne, G. D. (2005). Non-negative solutions of ODEs. *Applied Mathematics and Computation*, *170*(1), 556–569. https://doi.org/10.1016/j.amc.2004.12.011

Torlo, D., Öffner, P., & Ranocha, H. (2022). Issues with positivity-preserving Patankar-type schemes. *Applied Numerical Mathematics*, *182*, 117–147. https://doi.org/10.1016/j.apnum.2022.07.014

Zhu, F., Huang, J., & Yang, Y. (2024). Bound-preserving discontinuous Galerkin methods with modified Patankar time integrations for chemical reacting flows. *Communications on Applied Mathematics and Computation*, *6*(1), 190–217. https://doi.org/10.1007/s42967-022-00231-z