January 1, 2018

Dear SIAM Scientific Computing Editor(s),

On behalf of all authors, we would like to submit the manuscript, “Stability-Optimized Runge-Kutta Methods for Pathwise Stiffness in Stochastic Differential Equations”, for consideration. This work identifies a numerical issue for numerical stochastic differential equation solvers which we term pathwise stiffness. This property is characterized as the tendency for stochastic models to have random time points where large transient changes occur, like the switching between two steady states of a deterministically bistable model, making the model mostly non-stiff except for these small bursts of extreme stiffness. This is commonly seen in phenomenological models of biological systems and the resulting difficulty makes both traditional fixed time step explicit and implicit schemes inefficient.

In this manuscript we investigate four different methods to solve this common numerical issue. On one side, we derive adaptive strong order 1.5 explicit stochastic Runge-Kutta methods with enlarged stability regions, allowing as large as 5x the time steps of previous explicit methods while retaining the same efficiency on non-stiff problems. We show through numerical simulations that these methods can effectively handle the semi-stiff problems hundreds of times faster than common methods like Euler-Maruyama and Drift-Implicit Runge-Kutta Milstein schemes. Additionally, we derive adaptive strong order 1.5 L-stable implicit integrators, one a fully-implicit stochastic Runge-Kutta scheme and the other an extension of the Kennedy and Carpenter explicit first-stage singly diagonally implicit Runge-Kutta scheme (ESDIRK). While these implicit integrators are derived only for the case of additive noise, we show how the Lamperti transform can be used to extend the domain of solution to problems including mixed multiplicative and additive noise, which we term affine noise, which is the basis of most phenomenological noise models. Once again we demonstrate the efficiency of these new methods over previous implicit schemes. Additionally, the ESDIRK scheme is a stochastic extension of an additive Runge-Kutta scheme which can split the equation to treat different parts explicitly and implicitly. Our stochastic extension is compatible with the strong order 1.5 conditions on both the explicit and implicit parts. While we do not attempt to prove necessary conditions for strong order 1.5 IMEX schemes, we show a convergence test which demonstrates strong order 1.5 of the stochastic IMEX scheme on a nonlinear test equation. Lastly, we derive methods which allow for automated stiffness detection and demonstrate on a pathwise stiff equation that this method can accurately detect large transitions at a low computational cost. To our knowledge, these are the first high strong order adaptive implicit schemes for SDEs, the first adaptive IMEX scheme for SDEs, and the first demonstration of stiffness detection in SDEs.

Together, these four different routes form a strong toolset for tackling this common numerical issue for stochastic differential equations. In this manuscript we show biological models from recent literature where the efficiency difference changes the problem from seemingly computationally intractable to something which a standard desktop computer can solve. This has had a high impact on the scope of the biological models which are possible to research, and through this manuscript we hope to impact the toolsets of other stochastic modelers so they can see similar improvements.

**Suggested Reviewers**

Kevin Burrage ([kevin.burrage@qut.edu.au](mailto:kevin.burrage@qut.edu.au)), Queensland University of Science and Technology, expert in numerical methods for stochastic differential equations and biological modeling.

Pamela Burrage ([pamela.burrage@qut.edu.au](mailto:pamela.burrage@qut.edu.au)), Queensland University of Science and Technology, expert in numerical methods for stochastic differential equations and biological modeling.

Andreas Rößler ([roessler@math.uni-luebeck.de](mailto:roessler@math.uni-luebeck.de)), Universität zu Lübeck, expert in high order stochastic Runge-Kutta methods and adaptive time stepping for stochastic differential equations.

Peter Kloeden, ([kloeden@math.uni-frankfurt.de](mailto:kloeden@math.uni-frankfurt.de)), Goethe-Universität, expert in numerical methods for stochastic differential equations and biological modeling.

We look forward to hearing from you!

Sincerely Yours



Qing Nie

Professor of Mathematics, Biomedical Engineering, Developmental and Cell Biology