Stability-Optimized High Strong Order Methods for Stochastic Differential Equations with Additive and Diagonal Noise

Chris Rackauckas and Qing Nie

July 9, 2017

1 Introduction

Stochastic differential equations have seen increasing use in scientific fields such as biology and climate science due to their ability to capture the randomness inherent in physical systems. These equations are of the general form:

$$dX_t = f(t, X_t)dt + g(t, X_t)dW_t$$

where X_t is a d-dimensional vector, where $f : \mathbb{R}^d \to \mathbb{R}^d$ is the drift coefficient and $g : \mathbb{R}^d \to \mathbb{R}^{d\times m}$ is a matrix equation known as the diffusion coefficient which describes the amount and mixtures of the noise process W_t which is a m-dimensional Brownian motion. In many models, noise is added to deterministic equations phenomenologically. These models are numerically studied for their qualitatative behavior: scientists are interested not in numerical predictions exact to many decimal places but to understand the phonomena which only occurs in the presence of stochasticity, like random switching between cell types. In these cases, the noise process can be modeled as exogenous to the system and thus not dependent the system itself, leading to the assumption that $g(t, X_t) \equiv g(t)$ which is known as additive noise. Another common case is multiplicative noise, where to each deterministic equation a noise term $\sigma_i X_t^i dW_t$ is added to give proportional noise. This results in $g(t, X_t)$ being the diagonal matrix $\left(\sigma_i X_t^i\right)$ and thus falling into the more general category of diagonal noise.

The unique features of stochastic models in many cases are pathwise-dependent. The mean of a chemical reaction network may stay at a constant steady state, but in the presence of randomness this may be switching between various states. These pathwise properties are of interest because they capture the effects which cannot be found in deterministic models. However, these same effects exhibit numerical difficulties. Almost by definition these features exist in the single trajectories of the random processes and thus must be controlled individually. These trajectories display large, transient and random switching behavior which in a given trajectory causes stochastic bursts of numerical stiffness, a phonomena which we will denote pathwise stiffness. In previous work, the authors have shown that by using adaptive timestepping a stochastic reaction network of 19 reactants is able to be solve with an average timestep 100,000x larger than the value that was found necessary for stability. However, the methods were still largely "stability-bound", that is the tolerance was set to solve the model was determined by what was necessary for stability but was far below the error necessary for the application. The purpose of this investigation is to develop numerical methods with the ability to properly handle pathwise stiffness and allow for efficient solving of large Monte Carlo experiments. We approach this through two means. On one end we develop stability-optimized Stochastic Runge-Kutta (SRK) methods which have the property of having drastically enlarged stability regions. Similar to the Runge-Kutta Chebyschev (and the S-ROCK extension to the stochastic case), these methods are designed to be efficient for equations which display stiffness without fully commiting to implicit solvers. On the otherhand, to handle extreme stiffness we develop an implicit RK method for additive noise problems. We show that this method is A-L stable in a generalization of these terms to additive noise SDEs. To extend the utility of these methods, we derive and extension of the methods for additive SDEs to multiplicative SDEs through a transformation. In addition to the new methods, we display a novel scalable mechanism for the derivation of "optimal" Runge-Kutta methods, and use it to design stability-optimized methods for diagonal noise SDEs which would otherwise be analytically intractable due to the few million terms in the stability equation. Lastly, we show that on test problems that these methods are no less efficient than existing SRK methods when one only requires a few decimal places of accuracy ($> 10^{-6}$), but show that these methods have two to three times the stability region, allowing them to dramatically speed up computations on stability-bound problems.

2 Adaptive Strong Order 1.0/1.5 SRK Methods

The class of methods we wish to example are the Strong Order 1.5 SRK methods due to Rossler. The diagonal noise methods utilize the same general form and order conditions as the methods for scalar noise so we use their notation for simplicity. The strong order 1.5 methods for scalar noise are of the form

$$X_{n+1} = X_n + \sum_{i=1}^{s} \alpha_i f\left(t_n + c_i^{(0)} h, H_i^{(0)}\right) + \sum_{i=1}^{s} \left(\beta_i^{(1)} I_{(1)} + \beta_i^{(2)} \frac{I_{(1,1)}}{\sqrt{h}} + \beta_i^{(3)} \frac{I_{(1,0)}}{h} + \beta_i^{(4)} \frac{I_{(1,1,1)}}{h}\right) g\left(t_n + c_i^{(1)} h\right)$$

with stages

$$H_i^{(0)} = X_n + \sum_{j=1}^{s} A_{ij}^{(0)} f\left(t_n + c_j^{(0)} h, H_j^{(0)}\right) h + \sum_{j=1}^{s} B_{ij}^{(0)} g\left(t_n + c_j^{(1)} h, H_j^{(1)}\right) \frac{I_{(1,0)}}{h}$$

$$H_i^{(1)} = X_n + \sum_{j=1}^{s} A_{ij}^{(1)} f\left(t_n + c_j^{(0)} h, H_j^{(0)}\right) h + \sum_{j=1}^{s} B_{ij}^{(1)} g\left(t_n + c_j^{(1)} h, H_j^{(1)}\right) \sqrt{h}$$

where the I_j are the Wiktorsson approximations to the iterated stochastic integrals. In the case of additive noise, this reduces to the form

$$X_{n+1} = X_n + \sum_{i=1}^{s} \alpha_i f\left(t_n + c_i^{(0)} h, H_i^{(0)}\right) + \sum_{i=1}^{s} \left(\beta_i^{(1)} I_{(1)} + \beta_i^{(2)} \frac{I_{(1,0)}}{h}\right) g\left(t_n + c_i^{(1)} h\right)$$

with stages

$$H_i^{(0)} = X_n + \sum_{j=1}^{s} A_{ij}^{(0)} f\left(t_n + c_j^{(0)} h, H_j^{(0)}\right) h + \sum_{j=1}^{s} B_{ij}^{(0)} g\left(t_n + c_j^{(1)} h\right) \frac{I_{(1,0)}}{h}.$$

The tuple of coefficients $\left(A^{(j)}, B^{(j)}, \beta^{(j)}, \alpha\right)$ thus fully determine the SRK method. These coefficients are subject to the constraint equations:

The coefficients
$\left(A_0, B_0, \beta^{(i)}, \alpha\right)$ must satisfy the following order conditions to achieve order .5:

1. $\alpha^T e = 1$
2. $\beta^{(1)^T} e = 1$
3. $\beta^{(2)^T} e = 0$
4. $\beta^{(3)^T} e = 0$
5. $\beta^{(4)^T} e = 0$

additionally, for order 1:

1. $\beta^{(1)^T} B^{(1)} e = 0$
2. $\beta^{(2)^T} B^{(1)} e = 1$
3. $\beta^{(3)^T} B^{(1)} e = 0$
4. $\beta^{(4)^T} B^{(1)} e = 0$

and lastly for order 1.5:

1. $\alpha^T A^{(0)} e = \frac{1}{2}$
2. $\alpha^T B^{(0)} e = 1$
3. $\alpha^T \left(B^{(0)} e\right)^2 = \frac{3}{2}$
4. $\beta^{(1)^T} A^{(1)} e = 1$
5. $\beta^{(2)^T} A^{(1)} e = 0$
6. $\beta^{(3)^T} A^{(1)} e = -1$
7. $\beta^{(4)^T} A^{(1)} e = 0$
8. $\beta^{(1)^T} \left(B^{(1)} e\right)^2 = 1$
9. $\beta^{(2)^T} \left(B^{(1)} e\right)^2 = 0$
10. $\beta^{(3)^T} \left(B^{(1)} e\right)^2 = -1$
11. $\beta^{(4)^T} \left(B^{(1)} e\right)^2 = 2$
12. $\beta^{(1)^T} \left(B^{(1)} \left(B^{(1)} e\right)\right) = 0$
13. $\beta^{(2)^T} \left(B^{(1)} \left(B^{(1)} e\right)\right) = 0$
14. $\beta^{(3)^T} \left(B^{(1)} \left(B^{(1)} e\right)\right) = 0$
15. $\beta^{(4)^T} \left(B^{(1)} \left(B^{(1)} e\right)\right) = 1$

$$16. \ \frac{1}{2}\beta^{(1)^T} \left(A^{(1)} \left(B^{(0)} e\right)\right) + \frac{1}{3}\beta^{(3)^T} \left(A^{(1)} \left(B^{(0)} e\right)\right) = 0$$

where $f, g \in C^{1,2}(\mathcal{I} \times \mathbb{R}^d, \mathbb{R}^d)$, $c^{(i)} = A^{(i)} e$, $e = (1, 1, 1, 1)^T$. The reduced constraints for additive noise were derived for order 1:

1. $\alpha^T e = 1$
2. $\beta^{(1)^T} e = 1$
3. $\beta^{(2)^T} e = 0$

and the additional conditions for order 1.5:

1. $\alpha^T B^{(0)} e = 1$
2. $\alpha^T A^{(0)} e = \frac{1}{2}$
3. $\alpha^T \left(B^{(0)} e\right)^2 = \frac{3}{2}$
4. $\beta^{(1)^T} c^{(1)} = 1$
5. $\beta^{(2)^T} c^{(1)} = -1$

where $c^{(0)} = A^{(0)} e$ with $f \in C^{1,3}(\mathcal{I} \times \mathbb{R}^d, \mathbb{R}^d)$ and $g \in C^1(\mathcal{I}, \mathbb{R}^d)$.

Rackauckas and Nie showed that for any method of this form, there exists an error estimator

$$E = \delta E_D + E_N$$

where E_D is the deterministic (drift) error estimator and E_N is the noise error estimator, given respectively by

$$E_D = \left| h \sum_{i \in I_1} (-1)^{\sigma(i)} f\left(t_n + c_i^{(0)} h, H_i^{(0)}\right) \right|$$

$$E_N = \left| \sum_{i \in I_1} \left(\beta_i^{(3)} \frac{I_{(1,0)}}{h} + \beta_i^{(4)} \frac{I_{(1,1,1)}}{h} \right) g\left(t_n + c_i^{(1)} h, H_i^{(1)}\right) \right|$$

with some constraints on $\sigma(i)$ and the I_j. Thus unlike in the theory of ordinary differential equations, the choice of coefficients for SRK methods does not require explicitly finding an embedded method. This gives the means to extend any SRK method to an adaptive timestepping method which was shown to be fundamental for the transient behavior of pathwise stiffness.

3 Optimized-Stability High Order SRK Methods with Additive Noise

Using the terms as defined by Kloden and Platen, we define a discrete approximation as numerically stable if for any finite time interval $[t_0, T]$, there exists a positive constant Δ_0 such that for each $\epsilon > 0$ and each $\delta \in (0, \Delta_0)$

$$\lim_{\left|X_0^\delta - \bar{X}_0^\delta\right| \to 0} \sup_{t_0 \le t \le T} P\left(\left|X_t^\delta - \bar{X}_t^\delta\right| \ge \epsilon\right) = 0$$

where X_n^δ is a discrete time approximation with maximum step size $\delta > 0$ starting at X_0^δ and $\bar{X}_n^\delta$ respectively starting at $\bar{X}_n^\delta$. For additive noise, we consider the complex-valued linear test equations

$$dX_t = \mu X_t dt + dW_t$$

where λ is a complex number. In this framework, a scheme which can be written in the form

$$X_{n+1}^h = X_n^h G(\mu h) + Z_n^\delta$$

with a constant step size $\delta \equiv h$ and Z_n^δ are random variables which do not depend on the Y_n^δ, then the region of absolute stability is the set where for $z = \mu h$, $|G(z)| < 1$.

The additive SRK method can be written as

$$X_{n+1}^h = X_n^h + z\left(\alpha \cdot H^{(0)}\right) + \beta^{(1)} \sigma I_{(1)} + \sigma \beta^{(2)} \frac{I_{(1,0)}}{h}$$

where

$$H^{(0)} = \left(I - zA^{(0)}\right)^{-1} \left(\hat{X}_n^h + B^{(0)} e \sigma \frac{I_{(1,0)}}{h}\right)$$

where $\hat{X}_n^h$ is the size s constant vector of elements X_n^h and $e = (1,1,1,1)^T$. By substitution we receive

$$X_{n+1}^h = X_n^h \left(1 + z\left(\alpha \cdot \left(I - zA^{(0)}\right)^{-1}\right)\right) + \left(I - zA^{(0)}\right)^{-1} B^{(0)} e \sigma \frac{I_{(1,0)}}{h} + \beta^{(1)} \sigma I_{(1)} + \sigma \beta^{(2)} \frac{I_{(1,0)}}{h}$$

This set of equations decouples to the form of Equation ## since the iterated stochastic integral approximation I_j are random numbers and are independent of the X_n^h. Thus the stability condition is determined by the equation

$$G(z) = 1 + z\left(\alpha \cdot \left(I - zA^{(0)}\right)^{-1}\right).$$

3.1 Stability-Optimal 2-Stage Explicit SRA Methods

For explicit methods, the $A^{(i)}$ and $B^{(i)}$ are lower diagonal and we receive the simplified stability function

$$G(z) = 1 + A_{21}z^2\alpha_2 + z(\alpha_1 + \alpha_2)$$

for a two-stage additive noise SRK method. For this method we will find the method which optimizes the stability in the real part of z. Thus we wish to find $A^{(0)}, \alpha$ s.t. the negative real roots of $|G(z)| = 1$ are minimized. By the quadratic equation we see that there exists only a single negative root: $z = \frac{1-\sqrt{1+8\alpha_2}}{2\alpha_2}$. Using Mathematica's minimum function, we determine that the minimum value for this root subject to the order constraints is $z = \frac{3}{4}\left(1-\sqrt{\frac{19}{3}}\right) \approx -1.13746$. We see that this is achieved when $\alpha = \frac{2}{3}$, meaning that the SRA1 method due to Rossler achieves the maximum stability criteria. However, given extra degrees of freedom, we attempted to impose that $c_1^{(0)} = c_1^{(1)} = 0$ and $c_2^{(0)} = c_2^{(1)} = 1$ so that the error estimator spans the whole interval. This can lead to improved robustness of the adaptive error estimator. In fact, when trying to optimize the error estimator's span we find that there is no error estimator which satisfies $c_2^{(0)} > \frac{3}{4}$ which is the span of the SRA1 method. Thus the SRA1 is the stability-optimized 2-stage explicit method which achieves the most robust error estimator.

$$A^{(0)} = \begin{pmatrix} 0 & 0 \\ \frac{3}{4} & 0 \end{pmatrix},\quad B^{(0)} = \begin{pmatrix} 0 & 0 \\ \frac{3}{2} & 0 \end{pmatrix},\quad \alpha = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}$$
$$\beta^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix},\quad \beta^{(2)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix},\quad c^{(0)} = \begin{pmatrix} 0 \\ \frac{3}{4} \end{pmatrix},\quad c^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

3.2 Stability-Optimal 3-Stage Explicit SRA Methods

For the 3-stage SRA method, we recieve the simplified stability function

$$G(z) = A_{21}A_{31}\alpha_3 z^3 + A_{21}\alpha_2 z^2 + A_{31}\alpha_3 z^2 + A_{32}\alpha_3 z^2 + \alpha_1 z + \alpha_2 z + \alpha_3 z + 1$$

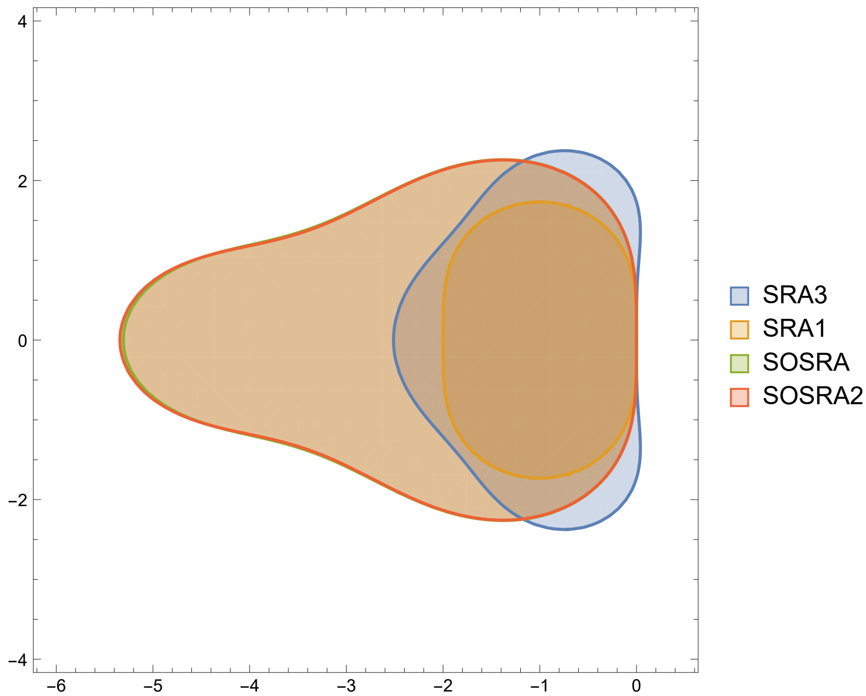
To optimize this method, we attempted to use the same techniques as before and optimize the real values of the negative roots. However, in this case we have a cubic polynomial and the root equations are more difficult. In the Mathematica notebooks we should that one root condition can be discarded, but the other two had difficulties optimizing. Instead, we turn to a more general technique to handle the stability optimization which will be employed in later sections as well. To do so, we generate an optimization problem which we can numerically solve for the coefficients. To simplify the problem, we let $z \in \mathbb{R}$. Define the function:

$$f(z, w; N, M) = \int_D \chi_{G(z)\leq 1}(z)dz$$

Notice that for $D \to \mathbb{C}$, f is the area of the stability region. Thus we define the stability-optimized diagonal SRK method as the set of coefficients which achieves

$$\max_{A^{(i)},B^{(i)},\beta^{(i)},\alpha} f(z)$$
$$\text{subject to: Order Constraints}$$

In all cases we impose $0 < c_i^{(0)}, c_i^{(1)} < 1$. We use the order constraints to simplify the problem to an nonlinear optimization problem on 14 variables with 3 equality constraints and 4 inequality constraints (with bound constraints on the 10 variables). However, we found that simplifying the problem even more to require $c_1^{(0)} = c_1^{(1)} = 0$ and $c_3^{(0)} = c_3^{(1)} = 1$ did not significantly impact the stability regions but helps the error estimator and thus we reduced the problem to 10 variables, 3 equality constraints, and 2 inequality constraints. This was optimized using the COBYLA local optimization algorithm with randomized initial conditions 100 times and all gave similar results. In the Mathematica notebook we show the effect of changing the numerical integration region D on the results, but conclude that a D which does not bias the result for better/worse real/complex handling does not improve the result. The resulting algorithm, SOSRA, we given by the coefficients in Table X in the appendix. Lastly, we used the condition that $c_2^{(0)} = c_3^{(0)} = c_2^{(1)} = c_3^{(1)} = 1$ to allow for free stability detection. The method generated with this extra constraint is SOSRA2. These methods have their stability regions compared to SRA1 and SRA3 in Figure X where it is shown that the SOSRA methods more than doubles the allowed real eigenvalues.



3.3 An A-Stable L-Stable 2-Stage (Semi-)Implicit SRA Method

It's clear that, as in the case for deterministic equations, the explicit methods cannot be made A-stable. However, the implicit two-stage additive noise SRK method is determined by

$$G(z) = \frac{z(A_{11}(A_{22}z - \alpha_2 z - 1) + A_{12}z(\alpha_1 - A_{21}) + A_{21}\alpha_2 z - A_{22}(\alpha_1 z + 1) + \alpha_1 + \alpha_2) + 1}{A_{11}z(A_{22}z - 1) - z(A_{12}A_{21}z + A_{22}) + 1}$$

which is A-stable if

$$A_{11}z(A_{22}z-1)-z(A_{12}A_{21}z+A_{22})+1 > z(A_{11}(A_{22}z-\alpha_2 z-1)+A_{12}z(\alpha_1-A_{21})+A_{21}\alpha_2 z-A_{22}(\alpha_1 z+1)+\alpha_1+\alpha_2)+1.$$

Notice that the numerator equals the denominator if and only if $z=0$ or

$$z=\frac{\alpha_1+\alpha_2}{\left(A_{22}-A_{12}\right)\alpha_1+\left(A_{11}-A_{21}\right)\alpha_2}.$$

From the order conditions we know that $\alpha_1+\alpha_2=1$ which means that no root exists with $Re(z)<0$ if $\left(A_{22}-A_{12}\right)\alpha_1+\left(A_{11}-A_{21}\right)\alpha_2>0$. Thus under these no roots conditions, we can determine A-stability by checking the inequality at $z=1$, which gives $1>\left(A_{22}-A_{12}\right)\alpha_1+\left(A_{11}-A_{21}\right)\alpha_2$. Using the order condition, we have a total of four constraints on the $A^{(0)}$ and α:

$$\begin{aligned}\left(A_{11}+A_{12}\right)\alpha_1+\left(A_{21}+A_{22}\right)\alpha_2&=\frac{1}{2}\\ \alpha_1+\alpha_2&=1\\ 0<\left(A_{22}-A_{12}\right)\alpha_1+\left(A_{11}-A_{21}\right)\alpha_2&<1\end{aligned}$$

An immediate fact we note is that none of the 2-stage (Order 3) Labatto or Radau methods create stochastically A-stable methods. Instead, we wish to derive methods which have similar properties and have stochastic A-stability. One property we extend is L-stability. The straightforward extension of L-stability is the condition

$$\lim_{z\to\infty}G(z)=0.$$

This implies that

$$\frac{-A_{11}A_{22}+A_{11}\alpha_2+A_{12}A_{21}-A_{12}\alpha_1-A_{21}\alpha_2+A_{22}\alpha_2\alpha_1}{A_{12}A_{21}-A_{11}A_{22}}=0$$

The denominator is $-\det(A^{(0)})$ which implies $A^{(0)}$ must be non-singular. Next, we attempt to impose B-stability on the drift portion of the method. We use the condition due to Burrage and Butcher that for $B=\operatorname{diag}\left(\alpha_1,\alpha_2\right)$ $M=BA^{(0)}+A^{(0)}B-\alpha\alpha^T$, we require both B and M to be non-negative definite. However, in the supplemental Mathematica notebooks we show computationally that there is no 2-stage SRK method of this form which satisfies all three of these stability conditions. Thus we settle for A-stability and L-stability.

Recalling that $c^{(0)}$ and $c^{(1)}$ are the locations in time where f and g are approximated respectively, we wish to impose

$$\begin{aligned}c_1^{(0)}&=0\\ c_2^{(0)}&=1\\ c_1^{(1)}&=0\\ c_2^{(1)}&=1\end{aligned}$$

so that the error estimator covers the entire interval of integration (for robustness to discontinuities). Since $c^{(0)}=A^{(0)}e$, this leads to the condition $A_{21}+A_{22}=1$. Using the constraint-satisfaction algorithm FindInstance in Mathematica, we look for tableaus which satisfy the previous conditions with the added constraint of semi-implicitness, i.e. $B^{(0)}$ is lower triangular. This assumption is added becaues the inverse of the normal distribution has unbounded moments, and thus in many cases it mathematically simpler to consider the diffusion term as explicit (though there are recent methods which drop this requirement via truncation or extra assumptions on the solution). However, we find that there is no coefficient set which meets all of these requirements. However, if we relax the interval estimate condition to allow $0 \leq c_2^{(0)} \leq 1$, we find an A-L stable method:

$$A^{(0)} = \begin{pmatrix} -1 & 1 \\ 0 & \frac{3}{4} \end{pmatrix}, \quad B^{(0)} = \begin{pmatrix} 0 & 0 \\ \frac{3}{2} & 0 \end{pmatrix}, \quad \alpha = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}$$
$$\beta^{(1)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \beta^{(2)} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad c^{(0)} = \begin{pmatrix} 0 \\ \frac{3}{4} \end{pmatrix}, \quad c^{(1)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

If we attempt to look for an SDIRK-like method to reduce the complexity of the implicit equation, i.e. $A_{12}^{(0)} = 0$, using FindInstance we find the constraints unsatisfiable. Note that if we drop the semi-implicit assumption we find that the full constraints cannot be satisfied there (we still cannot satisfy $c_1^{(0)} = 0$ and $c_2^{(0)} = 1$), and there does not exist an A-L stable SDIRK method in that case.

4 Optimized-Stability Methods for Multiplicative Noise via Transformation

Given the efficiency of the methods for additive noise, one method for developing efficient methods for more general noise processes is to use a transform of diagonal noise processes to additive noise. This transform is due to Lamperti, which states that the SDE of the form

$$dX_t = f(t, X_t)dt + \sigma(t, X_t)R(t)dW_t$$

where σ a diagonal matrix with diagonal elements $\sigma_i(t, X_{i,t})$ has the transformation

$$Z_{i,t} = \psi_i(t, X_{i,t}) = \int \frac{1}{\sigma_i(x,t)} dx \mid_{x=X_{i,t}}$$

which will result in an Ito process with the ith element given by

$$dZ_{i,t} = \left(\frac{\partial}{\partial t} \psi_i(t,x) \mid_{x=\psi^{-1}(t,Z_{i,t})} + \frac{f_i(\psi^{-1}(t,Z_t),t)}{\frac{1}{2}\frac{\partial}{\partial x}\sigma_i\left(\psi_i^{-1}\left(t,Z_{i,t}\right)\right)} \right) dt + \sum_{j=1}^{n} r_{ij}(t) dw_{j,t}$$

with

$$X_t = \psi^{-1}\left(t, Z_t\right).$$

This is easily verified using Ito's Lemma. An example of such a transformation is multidimensional geometric Brownian motion, where $A = diag(a_1, a_2)$, $\sigma = diag(X_1, X_2)$, and $R = r_{ij}$. Then in this case, $Z = \psi(X) = \log(X)$ and

$$d \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} = \begin{bmatrix} a_1 - \frac{1}{2}\left(r_{11}^2 + r_{12}^2\right) \\ a_2 - \frac{1}{2}\left(r_{21}^2 + r_{22}^2\right) \end{bmatrix} dt + \begin{bmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{bmatrix} dW_t.$$

This transformation requires that $\sigma_i^{-1}(t, X_{i,t})$ is one-to-one, and thus does not exist in general for diagonal noise. However, in the case of mixed multiplicative and additive noise:

$$dX_t = f(t, X_t)dt + \sigma X_t dW_t$$

where σ is a constant diagonal matrix, then

$$d\log X_t = \tilde{f}(t, X_t)dt + dW_t$$
$$\tilde{f}(t, X_t) = \frac{f(t, X_t)}{\sigma X_t}$$

where the division is considered element-wise. Thus we can modify the additive SRK method to be in the form

$$\log X_{n+1} = \log X_n + \sum_{i=1}^{s} \alpha_i \tilde{f}\left(t_n + c_i^{(0)}h, \exp\left(H_i^{(0)}\right)\right) + \sum_{i=1}^{s} \left(\beta_i^{(1)} I_{(1)} + \beta_i^{(2)} \frac{I_{(1,0)}}{h}\right)$$

with stages

$$H_i^{(0)} = \log X_n + \sum_{j=1}^{s} A_{ij}^{(0)} \tilde{f}\left(t_n + c_j^{(0)}h, \exp\left(H_j^{(0)}\right)\right) h + \sum_{j=1}^{s} B_{ij}^{(0)} \frac{I_{(1,0)}}{h}.$$

Back-transforming this, we get

$$X_{n+1} = X_n \exp\left(\sum_{i=1}^{s} \alpha_i \tilde{f}\left(t_n + c_i^{(0)}h, \exp\left(H_i^{(0)}\right)\right) + \sum_{i=1}^{s} \left(\beta_i^{(1)} I_{(1)} + \beta_i^{(2)} \frac{I_{(1,0)}}{h}\right)\right)$$

where the exponentiation is interpreted element-wise.

5 Optimized-Stability Order 1.5 SRK Methods with Diagonal Noise

5.1 The Stability Equation for Order 1.5 SRK Methods with Diagonal Noise

For diagonal noise, we will use the mean-square definition of stability. A method is mean-square stable if $\lim_{n\to\infty} \mathbb{E}\left(|X_n|^2\right) = 0$ on the test equation

$$dX_t = \mu X_t dt + \sigma X_t dW_t.$$

In matrix form we can re-write our method as given by

$$X_{n+1} = X_n + \mu h\left(\alpha \cdot H^{(0)}\right) + \sigma I_{(1)}\left(\beta^{(1)} \cdot H^{(1)}\right) + \sigma \frac{I_{(1,1)}}{\sqrt{h}}\left(\beta^{(2)} \cdot H^{(1)}\right) + \sigma \frac{I_{(1,0)}}{h}\left(\beta^{(3)} \cdot H^{(1)}\right) + \sigma \frac{I_{(1,1,1)}}{h}\left(\beta^{(4)} \cdot H^{(1)}\right)$$

with stages

$$\begin{aligned} H^{(0)} &= X_n + \mu\Delta t A^{(0)} H^{(0)} + \sigma \frac{I_{(1,0)}}{h} B^{(0)} H^{(1)}, \\ H^{(1)} &= X_n + \mu\Delta t A^{(1)} H^{(0)} + \sigma\sqrt{\Delta t} B^{(1)} H^{(1)} \end{aligned}$$

where $\hat{X_n}$ is the size s constant vector of X_n.

$$\begin{aligned} H^{(0)} &= \left(I - hA^{(0)}\right)^{-1}\left(\hat{X_n} + \sigma \frac{I_{(1,0)}}{h} B^{(0)} H^{(1)}\right), \\ H^{(1)} &= \left(I - \sigma\sqrt{h}B^{(1)}\right)^{-1}\left(\hat{X_n} + \mu h A^{(1)} H^{(0)}\right) \end{aligned}$$

By the derivation in the appendix, we receive the equation

$$
\begin{aligned}
S=E\left[\frac{U_{n+1}^{2}}{U_{n}^{2}}\right] = & \{1+\mu ht\left(\alpha\cdot\left[\left(I-\mu\Delta tA^{(0)}-\mu\sigma I_{(1,0)}A^{(1)}B^{(0)}\left(I-\sigma\sqrt{h}B^{(1)}\right)^{-1}\right)^{-1}\left(I+\sigma\frac{I_{(1,0)}}{h}B^{(0)}\left(I-\sigma\sqrt{h}B^{(1)}\right)^{-1}\right)\right]\right) \\
& +\sigma I_{(1)}\left(\beta^{(1)}\cdot\left[\left(I-\sigma\sqrt{h}B^{(1)}-\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{h}B^{(0)}\right)^{-1}\left(I+\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\right)\right]\right) \\
& +\sigma\frac{I_{(1,1)}}{\sqrt{h}}\left(\beta^{(2)}\cdot\left[\left(I-\sigma\sqrt{h}B^{(1)}-\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{h}B^{(0)}\right)^{-1}\left(I+\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\right)\right]\right) \\
& +\sigma\frac{I_{(1,0)}}{h}\left(\beta^{(3)}\cdot\left[\left(I-\sigma\sqrt{h}B^{(1)}-\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{h}B^{(0)}\right)^{-1}\left(I+\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\right)\right]\right) \\
& +\sigma\frac{I_{(1,1,1)}}{h}\left(\beta^{(4)}\cdot\left[\left(I-\sigma\sqrt{h}B^{(1)}-\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{h}B^{(0)}\right)^{-1}\left(I+\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\right)\right]\right)\}^{2}
\end{aligned}
$$

We apply the substitutions from the Appendix and let

$$
\begin{aligned}
z &= \mu h, \\
w &= \sigma\sqrt{h}.
\end{aligned}
$$

In this space, z is the stability variable for the drift term and w is the stability in the diffusion term. Under this scaling $\left(h,\sqrt{h}\right)$, the equation becomes independent of h and thus becomes a function $S(z,w)$ on the coefficients of the SRK method. The equation $S(z,w)$ in terms of its coefficients for explicit methods ($A^{(i)}$ and $B^{(i)}$ lower diagonal) has millions of terms and is shown in the supplemental Mathematica notebook. Determination of the stability equation for the implicit methods was found to be computationally intractable and is an avenue for further research.

5.2 An Optimization Problem for Determination of Coefficients

We wish to determine the coefficients for the additive and diagonal SRK methods which optimize the stability. To do so, we generate an optimization problem which we can numerically solve for the coefficients. To simplify the problem, we let $z,w\in\mathbb{R}$. Define the function

$$
f\left(z,w;N,M\right)=\int_{-M}^{M}\int_{-N}^{1}\chi_{S(z,w)\leq1}(z,w)dzdw.
$$

Notice that for $N,M\rightarrow\infty$, f is the area of the stability region. Thus we define the stability-optimized diagonal SRK method as the set of coefficients which achieves

$$
\begin{gathered}
\max_{A^{(i)},B^{(i)},\beta^{(i)},\alpha} f(z,w) \\
\text{subject to: Order Constraints}
\end{gathered}
$$

However, like with the SRK methods for additive noise, we impose a few extra constraints to add robustness to the error estimator. In all cases we impose $0<c_i^{(0)},c_i^{(1)}<1$. Additionally we can prescribe $c_4^{(0)}=c_4^{(1)}=1$ which we call the End-C Constraint. Lastly, we can prescribe the ordering constraint $c_1^{(j)}<c_2^{(j)}<c_3^{(j)}<c_4^{(j)}$ which we denote as the Inequality-C Constraint.

The resulting problem is a nonlinear programming problem with 44 variables and 42-48 constraint equations. The objective function is the two-dimensional integral of a discontinuous function which is determined by a polynomial of in z and w with approximately 3 million coefficients. To numerically approximate this function, we calculated the characteristic function on a grid with even spacing dx using a CUDA kernel and found numerical solutions to the optimization problem using the JuMP framework with the NLopt backend. A mixed approach using many solutions of the semi-local optimizer LN_AUGLAG_EQ and fewer solutions from the global optimizer GN_ISRES were used to approximate the optimality of solutions. Optimization was run many times in parallel until many results produced methods with similar optimiality, indicating that we were likely obtained values near the true minimum.

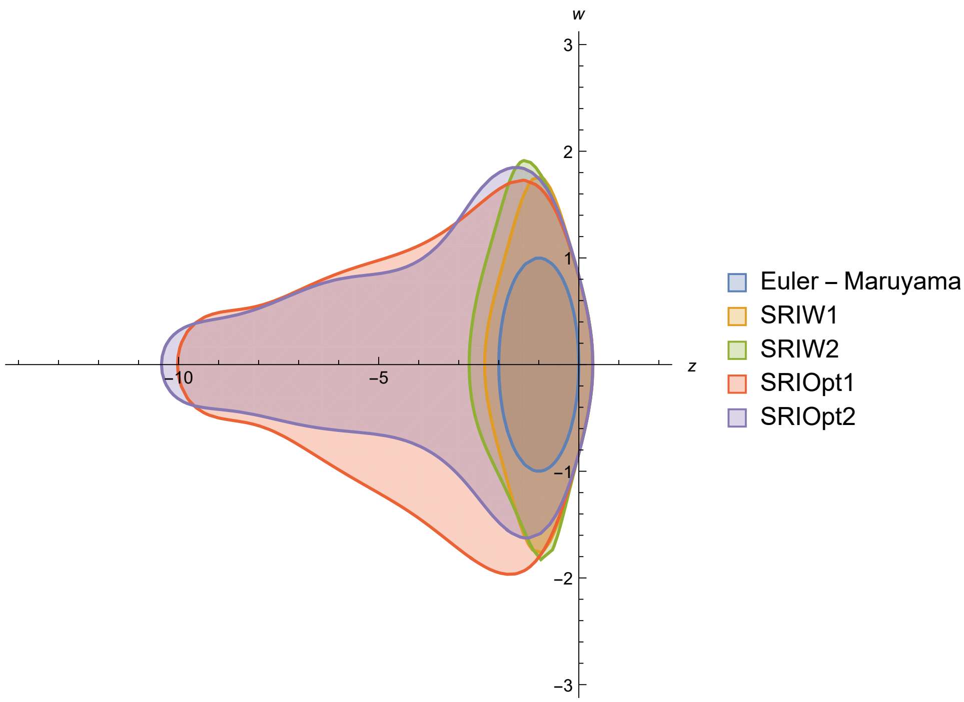
The parameters N and M are the bounds on the stability region, but also represent a tradeoff between the stability in the drift and the stability in the diffusion. A method which is optimized when M is small would be highly stable in the case of small noise, but would not be guaranteed to have good stability properties in the presence of large noise. Thus these parameters are knobs for tuning the algorithms for specific situations, and thus we solved the problem for different combinations of N and M to determine different algorithms for the different cases.

5.3 Resulting Approximately-Optimal Methods

The coefficients generated for approximately-optimal methods fall into three categories. In one category we have the drift-dominated stability methods where large N and small M was optimized. On the other end we have the diffusion-dominated stability methods where large M and small N was optimized. Then we have the mixed stability methods which used some mixed size choices for N and M. As a baseline, we optimized the objective without constraints on the c_i to see what the "best possible method" would be. When this was done with large N and M, the resulting method, which we name SRIOpt1, has almost every value of c satisfy the constraints, but with $c_2^{(0)} \approx -0.04$ and $c_4^{(0)} \approx 3.75$. To see if we could produce methods which were more diffusion-stable, we decreased N to optimize more in w but failed to produce methods with substantially enlarged diffusion-stability over SRIOpt1.

Adding only the inequality constraints on the c_i and looking for methods for drift-dominated stability, we failed to produce methods whose c_i estimators adequately covered the interval. Some of the results did produce stability regions simliar to SRIOpt1 but with $c_i^{(0)} < 0.5$ which indicates the method could have problems with error estimation. When placing the equality constraints on the edge c_i, one method, which we label SRIOpt2, resulted in similar stability to SRIOpt1 but satisfy the c_i constraints. In addition, this method satisfies $c_3^{(0)} = c_4^{(0)} = 1$ and $c_3^{(1)} = c_4^{(1)} = 1$, a property whose use will be explained in Section X.

To look for more diffusion-stable methods, we dropped to $N = 6$ to encourage the methods to expand the stability in the w-plane. However, we could not find a method whose stability region went substantially beyond $[-2, 2]$ in w. This was further decreased to $N = 1$ where methods still could not go substantially beyond $|2|$. Thus we were not able to obtain methods optimized for the diffusion-dominated case. This hard barrier was hit under many different constraint and objective setups and under thousands of optimization runs, indicating there might be a diffusion-stability barrier for explicit methods.



5.4 Approximately-Optimal Methods with Stability Detection and Switching Behaviors

In many real-world cases, one may not be able to clearly identify a model as drift-stability bound or diffusion-stability bound, or if the equation is stiff or non-stiff. In fact, many models may switch between such extremes. An example is a model with stochastic switching between different steady states. In this case, we have that the diffusion term $f(t, X_{ss}) \approx 0$ in the area of many stochastic steady states, meaning that while straddling a steady state the integration is heavily diffusion-stability dominated and usually non-stiff. However, when switching between steady states, f can be very large and stiff, causing the integration to be heavily drift-stability dominated. Since these switches are random, the ability to adapt between these two behaviors could be key to achieving optimal performance. Given the tradeoff, we investigated how our methods allow for switching between methods which optimize for the different situations.

The basis for our method is a straight-forward extension of a method proposed for deterministic differential equations. The idea is to create a cheap approximation to the dominant eigenvalues of the Jacobians for the drift and diffusion terms. If v is the eigenvector of the respective Jacobian, then for $\|v\|$ sufficiently small,

$$|\lambda_D| \approx \frac{\|f(t, x+v) - f(t,x)\|}{\|v\|}, \quad |\lambda_N| \approx \frac{\|g(t, x+v) - g(t,x)\|}{\|v\|}$$

where $|\lambda_D|$ and $|\lambda_N|$ are the estimates of the dominant eigenvalues for the deterministic and noise functions respectively. We have in approximation that $H_i^{(k)}$ is an approximation for $X_{t+c_i^{(k)}h}$ and thus the difference between two successive approximations at the same timepoint, $c_i^{(k)} = c_j^{(k)}$, then the following serves as a local Jacobian estimate:

$$|\lambda_D| \approx \frac{\|f(t+c_i^{(0)}h, H_i^{(0)}) - f(t+c_j^{(0)}h, H_j^{(0)})\|}{\|H_i^{(0)} - H_j^{(0)}\|}, \quad |\lambda_N| \approx \frac{\|f(t+c_i^{(1)}h, H_i^{(1)}) - f(t+c_j^{(1)}h, H_j^{(1)})\|}{\|H_i^{(1)} - H_j^{(1)}\|}$$

If we had already computed a successful step, we would like to know if in the next calculation we should switch methods due to stability. Thus it makes sense to approximate the Jacobian at the end of the interval, meaning $i = s$ and $j = s - 1$ where s is the number of stages. Then if z_{min} is the minimum $z \in \mathbb{R}$ such that z is in the stability region for the method, $\frac{h|\lambda_D|}{z_{min}} > 1$ when the steps are outside the stability region. Because the drift and mixed stability methods do not track the noise axis directly, we instead modify w_{min} to be $\frac{2}{3}$ of the maximum of the stability region in the noise axis.

Hairer noted that, for ODEs, if a RK method has $c_i = c_j = 1$, then it follows that

$$\rho = \frac{\|k_i - k_j\|}{\|g_i - g_j\|}$$

where $k_i = f(t + c_i h, g_i)$ is an estimate of the eigenvalues for the Jacobian of f. Given the construction of SRIOpt2, a natural extension is

$$|\lambda_D| \approx \frac{\|f\left(t_n + c_4^{(0)}h, H_4^{(0)}\right) - f\left(t_n + c_3^{(0)}h, H_3^{(0)}\right)\|}{\|H_4^{(0)} - H_3^{(0)}\|}, \quad |\lambda_N| \approx \frac{\|g\left(t_n + c_4^{(0)}h, H_4^{(1)}\right) - g\left(t_n + c_3^{(0)}h, H_3^{(1)}\right)\|}{\|H_4^{(1)} - H_3^{(1)}\|}$$

Given that these values are all part of the actual step calculations, this stiffness estimate is free. By comparing these values to the stability plot in Figure X, we use the following heristic to decide if SRIOpt2 is stability-bound in its steps:

1. If $10 > |\lambda_D| > 2.5$, then we check if $h\,|\lambda_N| > 1$.
2. If $|\lambda_D| < 2.5$, then we check if $h\,|\lambda_N|/2 > 1$.

The denominator is chosen as a reasonable approximation to the edge of the stability region. If either of those conditions are satisfied, then h is constrained by the stability region. The solver can thus alert the user that the method is non-stiff or use this estimate to switch to a method more suitable for stiff equations. In addition, the error estimator gives separate error estimates in the drift and diffusion terms. A scheme could combine these two facts to develop a more robust stiffness detection method, and label the stiffness as either drift or diffusion dominated.

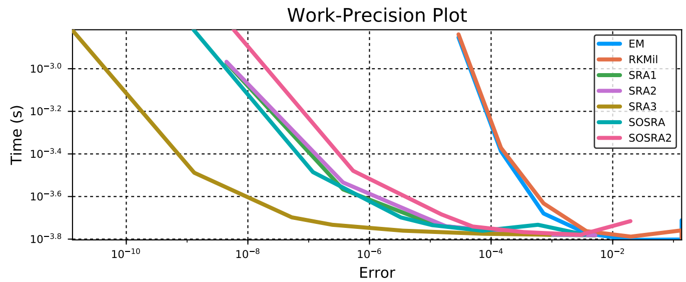
We end by noting that SRSRA2 has the same property, allowing stiffness detection via

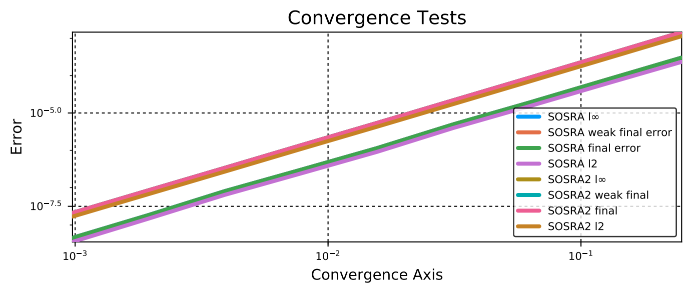
$$|\lambda_D| \approx \frac{\|f\left(t_n + c_3^{(0)}h, H_3^{(0)}\right) - f\left(t_n + c_2^{(0)}h, H_2^{(0)}\right)\|}{\|H_3^{(0)} - H_2^{(0)}\|}$$

and, employing a similar method as the deterministic case, check for stiffness via the estimate $h\,|\lambda_D|/5 > 1$.

6 Numerical Results

6.1 SOSRA Numerical Experiments





6.2 SOSRI Numerical Experiments

- Efficiency on Oval2 problem?

7 Discussion

- non-commutative and commutative
- principle truncation

8 Appendix: Derivations

$$
\begin{aligned}
\left(I-\mu\Delta tA^{(0)}\right)H^{(0)} &= U_n+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\left(U_n+\mu\Delta tA^{(1)}H^{(0)}\right), \\
\left(I-\mu\Delta tA^{(0)}\right)H^{(0)}-\left[\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\right]\mu\Delta tA^{(1)}H^{(0)} &= U_n+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}U_n \\
\left(I-\mu\Delta tA^{(0)}-\mu\Delta tA^{(1)}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\right)H^{(0)} &= \left(I+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\right)U_n \\
H^{(0)} &= \left(I-\mu\Delta tA^{(0)}-\mu\sigma I_{(1,0)}A^{(1)}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\right)^{-1}\left(I+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1}\right.\right.
\end{aligned}
$$

$$
\begin{aligned}
\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)H^{(1)} &= U_n+\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\left(U_n+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}H^{(1)}\right)\\
\left(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)H^{(1)} &= U_n+\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}U_n\\
\left(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)H^{(1)} &= \left(I+\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\right)U_n\\
H^{(1)} &= \left(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I+\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\right)U
\end{aligned}
$$

$$
\begin{aligned}
U_{n+1} = {} & U_n+\mu\Delta t\left(\alpha\cdot\left[\left(I-\mu\Delta tA^{(0)}-\mu\sigma I_{(1,0)}A^{(1)}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\right)^{-1}\left(I+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\left(I-\sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\right)\right]U_n\right)\\
& +\sigma I_{(1)}\left(\beta^{(1)}\cdot\left[\left(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I+\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\right)\right]U_n\right)\\
& +\sigma\frac{I_{(1,1)}}{\sqrt{\Delta t}}\left(\beta^{(2)}\cdot\left[\left(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I+\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\right)\right]U_n\right)\\
& +\sigma\frac{I_{(1,0)}}{\Delta t}\left(\beta^{(3)}\cdot\left[\left(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I+\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\right)\right]U_n\right)\\
& +\sigma\frac{I_{(1,1,1)}}{\Delta t}\left(\beta^{(4)}\cdot\left[\left(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I+\mu\Delta tA^{(1)}\left(I-\mu\Delta tA^{(0)}\right)^{-1}\right)\right]U_n\right)
\end{aligned}
$$

Thus we substitute in the Wiktorsson approximations

$$
\begin{aligned}
I_{(1,1)} &= \frac{1}{2}\left(\Delta W^2-h\right)\\
I_{(1,1,1)} &= \frac{1}{6}\left(\Delta W^3-3h\Delta W\right)\\
I_{(1.0)} &= \frac{1}{2}h\left(\Delta W+\frac{1}{\sqrt{3}}\Delta Z\right)
\end{aligned}
$$

where $\Delta Z\sim N(0,h)$ is independent of $\Delta W\sim N(0,h)$. By the properties of the normal distribution, we have that

$$
E\left[(\Delta W)^n\right]=0
$$

for any odd n and

$$
\begin{aligned}
E\left[(\Delta W)^2\right] &= h\\
E\left[(\Delta W)^4\right] &= 3h^2\\
E\left[(\Delta W)^6\right] &= 15h^3\\
E\left[(\Delta W)^8\right] &= 105h^4.
\end{aligned}
$$