

The fully implicit stochastic- α method for stiff stochastic differential equations [☆]

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ABSTRACT

A fully implicit integration method for stochastic differential equations with significant multiplicative noise and stiffness in both the drift and diffusion coefficients has been constructed, analyzed and illustrated with numerical examples in this work. The method has strong order 1.0 consistency and has user-selectable parameters that allow the user to expand the stability region of the method to cover almost the entire drift-diffusion stability plane. The large stability region enables the method to take computationally efficient time steps. A system of chemical Langevin equations simulated with the method illustrates its computational efficiency.

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1. Introduction

Many models in physics yield stochastic differential equations (SDEs) with multiplicative noise. Consequently along with the drift coefficient the diffusion coefficients too contribute to the (sample pathwise) stiffness (in the sense of sharp changes in a small time scale [10]) of the SDE. A few examples [34,29,2,14,4,15] are the hydrology models, the Langevin equations of chemical physics and the models for laser emission. For numerical integration of stiff SDEs with multiplicative noise, the stiffness in diffusion coefficients has necessitated the development of fully implicit numerical integration schemes. However, a straightforward formulation of a fully implicit scheme faces the problem of being stochastic unstable [1,15]. Hence balanced implicit methods ([20,12,23–25,6,4,15,27] and references therein) have been constructed. The stability regions of the balanced implicit methods, although sufficient for simulation of many SDE models, are not large enough (cf. Fig. 6.2 in [32]) for admitting efficient (i.e., largest possible time step that meets physically acceptable mean square accuracy requirements) time step sizes in problems where the stiffness in the diffusion coefficients is comparable to or computationally more significant than that in the drift coefficients. This difficulty has been explained and pointed out in [16] since many physical systems (e.g., the chemical Langevin equations) [29,34] are characterized by computationally significant stiffness in the diffusion coefficients. To address this difficulty with the stability region, in the present work we construct a balanced implicit Milstein scheme [18,20] with a stability region that can cover almost the entire drift-diffusion plane in mean square stability (cf. Figs. 6.2 and 6.3 later in this work). The present scheme handles stiffness by providing numerical dissipation in both the drift and the diffusion terms. The construction of the numerical scheme in this work draws upon the generalized α method for deterministic stiff ordinary differential equations (ODEs) [35,17,8] for the definition of its parameters and for its structure. However any similarity or connection with its deterministic counterpart ends here due to the Itô stochastic

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calculus involved. A drift implicit Stochastic- α method was developed in [21] and the effect of the diffusion terms on the stability of the method was analyzed. The time step size of the drift implicit method in [21] decreases rapidly when stiffness in the diffusion becomes computationally significant. Hence the present development of a fully implicit version of the Stochastic- α method.

2. Initial value stochastic differential equation

Let there be a common underlying complete probability space $(\Omega, \mathcal{A}, \mathbf{P})$ with index $t \in \mathcal{T} := [t_0, t_f] \subset \mathbb{R}$ on which the vector stochastic process $x(t)$ consists of component-wise collections of random variables. Along a given sample path ω , $x(t; \omega)$ denotes the value taken by the random variable x_t . We consider the numerical integration of the initial value Itô SDE with multiplicative noise in the form of

$$dx = f(x, t)dt + \sum_{j=1}^m b^{(j)}(x, t)dW_t^{(j)} \quad \text{with} \quad (2.1)$$

$$\mathbf{P}(x(t_0) = x_0) = 1 \quad (\text{i.e., almost surely } x(t_0) = x_0) \quad (2.2)$$

where $x_t \in \mathbb{R}^l$ with probability 1, $f: \mathbb{R}^l \times \mathcal{T} \rightarrow \mathbb{R}^l$ and each $b^{(j)}: \mathbb{R}^l \times \mathcal{T} \rightarrow \mathbb{R}^l$, $t \in \mathcal{T}$, $j = 1, \dots, m$ are respectively the deterministic drift and diffusion coefficient (corresponding to the j th component of the Wiener process) functions in x, t ; $W_t^{(j)}$ is the j th component of the component-wise independent m -dimensional vector Wiener process W at time t .

2.1. Stiffness in diffusion and numerical methods

The computational significance of the stiffness in the diffusion coefficient and its effect on the stability of numerical integration of SDEs with multiplicative noise have been analyzed in the following references. In this section we denote a numerically computed $x(t_n; \omega)$ as x_n .

- (a) In [24] SDEs with single channel multiplicative noise of the form $dx_t = \lambda x_t dt + \mu x_t dW_t$, where $\lambda, \mu \in \mathbb{C}$ with $\Re(\lambda) < 0$ are considered. The Milstein scheme (for one-dimensional Wiener process) [18] $x_{n+1} = x_n + \lambda x_n h + \mu x_n \Delta W_n + \frac{(\Delta W_n)^2 - h}{2} \mu^2 x_n$ where h is the time step size and $\Delta W_n := W_{n+1} - W_n$ is the Wiener process increment over the n th time step, having $O(h^{1.5})$ root mean-square error, is analyzed for its stability in the mean square sense. The mean square stability function $R(h) = |1 + h\lambda|^2 + |h\mu|^2 + \frac{1}{2}|h^2 \mu^4|$ is derived and it is shown that the SDE is asymptotically stochastic stable in the mean square when $R(h) < 1$. The mean square stability and choice of time step size for a few well-known numerical methods for integrating a test SDE with multiplicative noise are also studied in [24].
- (b) In [25] vector SDEs with single channel multiplicative noise of the form $dx_t = D x_t dt + \bar{B} x_t dW_t$, where $D = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$ and $\bar{B} = \begin{pmatrix} \alpha_1 & \beta_1 \\ \beta_2 & \alpha_2 \end{pmatrix}$ have been analyzed for their mean square stability. It is shown that the above SDE is mean square stable in the ∞ norm if $\max\{2\lambda_1 + (|\alpha_1| + |\beta_1|)^2, 2\lambda_2 + (|\alpha_2| + |\beta_2|)^2\} < 0$.
- (c) In [12], a test equation with multiplicative noise discretized with the stochastic Theta method is analyzed for its mean square and asymptotic stability.
- (d) The results of [24] generalize those of [12], and conditions akin to deterministic $A(\alpha)$ stability are examined in [11]. The stochastic Theta method for SDEs with squared diffusion coefficients upper bounded as twice the drift, is shown to recover A -stability like mean square stability for a parameter value greater than $3/2$ which is beyond its usual range for the deterministic Theta method.

2.2. Balanced implicit methods

Next, we review the significant developments in fully implicit methods for numerically integrating SDEs that have stiffness in both drift and diffusion.

- (e) The balanced implicit scheme of [19] discretizes the SDE (2.1) and (2.2) on a uniform mesh over the simulation interval $[t_0, t_f]$ as follows for the n th time step:

$$x_{n+1} = x_n + f(x_n, t_n) + \sum_{j=1}^m b^{(j)}(x_n, t_n) \Delta W_n^{(j)} + C_n(x_n - x_{n+1}),$$

where

$$C_n = c_0(x_n, t_n)h + \sum_{j=1}^m c_j(x_n, t_n) |\Delta W_n^{(j)}|,$$

$\Delta W_n^{(j)} = W_{t_{n+1}}^{(j)} - W_{t_n}^{(j)}$, and $h = t_{n+1} - t_n, n \in \{0, 1, \dots, N - 1\}$ and c_0, c_1, \dots, c_m represent $d \times d$ matrix valued functions. It is assumed that for any sequence of real numbers $\alpha_i, i = 1, \dots, m$ with $\alpha_0 \in [0, \bar{\alpha}], \alpha_1 \geq 0, \dots, \alpha_m \geq 0, \bar{\alpha} \geq h$ for all time step sizes h and $(t, x) \in [0, \infty] \times \mathbb{R}^d$, the matrix

$$M(x, t) := \mathcal{I} + \alpha_0 c_0(x, t) + \sum_{j=1}^m \alpha_j c_j(x, t), \quad (\mathcal{I} \text{ being the identity matrix}),$$

has an inverse and satisfies the condition

$$\|M(x, t)^{-1}\| \leq K < \infty.$$

- (f) In [1], the scheme $x_{n+1} = x_n + hf(x_n, t_n) + \sum_{j=1}^d \Delta W_n^{(j)} b^{(j)}(x_n, t_n) + D_n(x_n - x_{n+1})$ is considered, where the $m \times m$ matrix D_n is given by $D_n = hd_0(x_n, t_n) + \sum_{j=1}^m |\Delta W_n^{(j)}| d_j(x_n, t_n)$, and $d_j, j = 0, \dots, m$ are, in general, matrix valued functions which are often chosen as constants. The balanced method

$$x_{n+1} = x_n + (\mathcal{I} + D_n)^{-1} (hf(x_n, t_n) + \sum_{j=1}^m \Delta W_n^{(j)} b^{(j)}(x_n, t_n)),$$

where D_n acts as a damping factor, is then developed.

- (g) In [13], a numerical scheme that represents a class of linear-implicit schemes is developed. These schemes generate implicit numerical approximations with some qualitative improvements on the balanced implicit methods of [19,1] while obtaining a global $O(h)$ root mean square convergence. Similar methods along with numerical applications can be found in [9].
- (h) More recently the Modified split-step backward balanced Milstein method (MSSBBM) has been described in [32] for a single noise system under the same assumptions as in [12,24]:

$$y_n = x_n + h(f(y_n, t_n) - \frac{1}{2} b^{(1)}(y_n, t_n))$$

$$x_{n+1} = y_n + \Delta W_n b^{(1)}(y_n, t_n) + \frac{1}{2} \frac{\partial}{\partial x} b^{(1)}(y_n, t_n) b^{(1)}(y_n, t_n) (\Delta W_n)^2 + C_n (y_n - x_{n+1}),$$

where $C_n = c_0(x_n, t_n)h + c_2(x_n, t_n)[(\Delta W_n)^2 - h]$ with $c_2 > 0$ and $c_0 - c_2 > 0$.

All of the above methods are able to numerically integrate many classes of stiff SDEs with multiplicative noise. However, the mean square stability region (Figs. 6.1 and 6.2 in [32]) for each of these methods, only slightly improving on the older method, is deficient in covering systems where the stiffness in the diffusion coefficients is comparable to or more significant compared to that in the drift and consequently the time step taken by the above methods must become extremely small (as is seen from the mean square stability plots in Figs. 6.1 and 6.2 in [32]) leading to computational inefficiency.

2.3. Other methods for stiff SDEs

Apart from the balanced implicit schemes, local linearization (e.g., as in [22,7]) is another technique that has been attempted to ease the difficulty arising from stiffness in SDEs. But these methods have the limitation that the error and stability of the transformed random differential equation (RDE) which is solved at each time step depend on where and how the linearization is done. Finding the trade-off between error and stability for the linearization is not trivial for most applications. Hence the application of these methods are confined to SDEs with very specific structure, such as SDEs with linear commutative noise [7].

Adaptive time stepping schemes aim to restrict the extremely small time steps only over the subinterval of the simulation interval where the SDE is very stiff. In [29] an adaptive time stepping scheme with a modification of the Milstein method (but not a balanced implicit Milstein method) has been considered and involves the extra work in error estimation and mesh refinement which can be inefficient if the SDE is stiff over a large subinterval of the simulation interval. In [29] it may also be seen that such schemes can have large variance, requiring very large number of Monte-Carlo simulations for establishing a practical confidence interval for mean behavior of the solution. In [5] the adaptive time stepping is used with balanced implicit methods for taking smaller time steps with SDEs driven primarily by stiff multiplicative noise thus overcoming to large extent the numerical stability problem. In the present method we obtain an expanded stability region which makes the fully implicit method robust to the choice of relatively larger and more efficient time step sizes. This, in turn, reduces the overall computational effort over a given sample path.

3. Assumptions

Without loss of generality for computational purposes, we make the following standard assumptions as found on pp. 128–129 of [15]. A mathematical treatment explaining the assumptions can be found in [27,28].

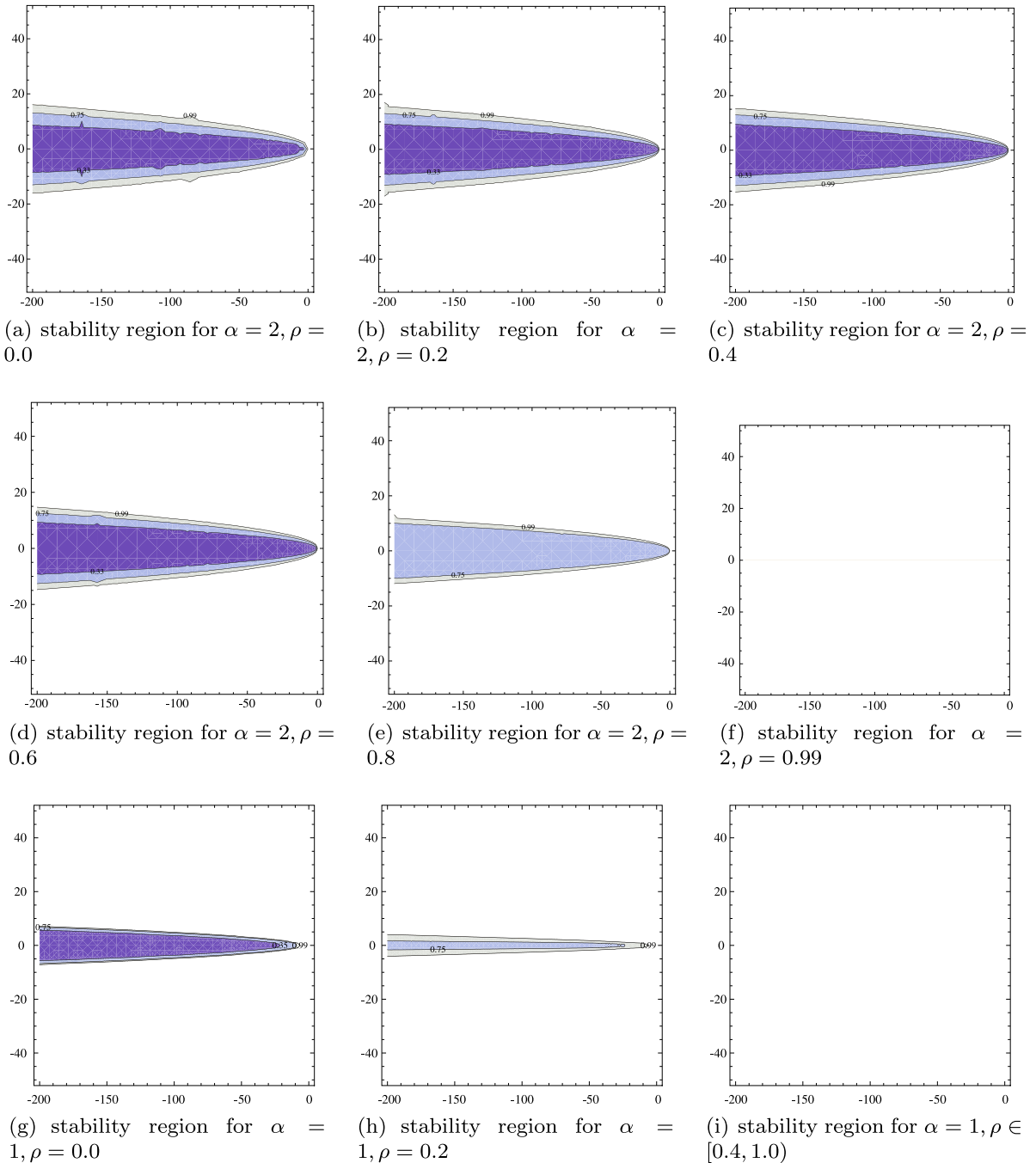


Fig. 6.1. The stability regions for $\alpha = 1.0, 2.0$ with various ρ 's are the contour plots of the integral $s_{\rho,2.0}$ in (6.5). The horizontal axis is $\lambda \in [-200.0, 0.0]$ and the vertical axis is $\eta \in [-50.0, 50.0]$. The white spaces in the contour plots of the integral $s_{\rho,\alpha}$ in (6.5) are excluded from the stability regions. The dark shaded region corresponds to the values of the integral $s_{\rho,\alpha}$ in (6.5) being in $[0.0, 0.33]$, the medium shaded region to values in $[0.33, 0.75]$ and the lightly shaded region corresponds to $[0.75, 0.99]$. It may be noted by comparing with Fig. 6.2 in [32] that the stability region for $\rho = 0.0, \alpha = 2.0$ roughly envelopes the union of the stability region of the existing balanced implicit methods.

- A1. *Regularity.* The functions $f, b^{(j)}$ (for $j = 1, \dots, m$) and the process $x(t)$ are assumed to be sufficiently regular.
- A2. *Non-anticipativity.* The process $x(t)$ is adapted to $\{\mathcal{A}_t, t \geq t_0\}$ which is the family of complete sub- σ -algebras (filtration) (of the σ -algebra \mathcal{A}) associated with W_t . This makes $x(t)$ non-anticipative to W_t .
- A3. *Continuity and Differentiability.* The functions f and $b^{(j)}$ for $j = 1, \dots, m$, all of which are deterministic functions of x, t are sufficiently and continuously (partial) differentiable with respect to x, t . The coefficients and the components of their partial derivatives (up to a sufficient order) are jointly L^2 -measurable in $(x^T, t)^T$ and are uniformly Lipschitz in $(x^T, t)^T$ over the sets of values taken during the integration of the initial value SDE (2.1) over $[t_0, t_f]$.

- A4. *Linear Growth Bound.* Each component of $b^{(j)}$ for $j = 1, \dots, m$ and f and their partial derivatives up to a sufficient order satisfy the linear growth upper bound of $(K_{l_1} + K_{l_2} \|x\|^2)$ in the mean square, where the K 's are suitable positive constants.
- A5. *Initial Value.* The initial value $x(t_0)$ is \mathcal{A}_{t_0} -measurable with $E(\|x(t_0)\|^2) < \infty$.
- A6. *A priori Estimate.* The *a priori* estimate that $\max_{n \in \{0, \dots, N\}} E\|x_n\|^{2q} < \infty$ for $q = 1, 2, \dots$ holds at the nodal points in a mesh partitioning $[t_0, t_f]$ into N time steps.

4. The fully implicit stochastic- α (FIS- α) method

In this section we describe the fully implicit stochastic- α FIS- (α) method for solving the initial value SDE problem (2.1) on a uniform mesh $t_0 < t_1 < \dots < t_n < t_{n+1} < \dots < t_N = t_f$ of time step size $t_{n+1} - t_n := h$ on the simulation interval $[t_0, t_f]$ which is normalized to $[0, 1]$. We denote a numerically computed value of $x(t_n; \omega)$ on a given sample path ω as x_n . The numerically computed x at a time point along a given sample path is distinguished from its analytical representation by the integer subscript as its index as opposed to the real index on its analytical representation. Let

$$\begin{aligned} \Delta W_n &:= \int_{t_n}^{t_{n+1}} dW_s; I_{(j_1 j_2)_n} = \int_{t_n}^{t_{n+1}} \int_{t_n}^s dW_u^{(j_1)} dW_s^{(j_2)} \\ B(x, t) &:= \{b^{(1)}, \dots, b^{(m)}\} : \mathbb{R}^l \times \mathcal{T} \rightarrow \mathbb{R}^{l \times l} \\ \nabla^{(i)} &:= \frac{\partial}{\partial x^{(i)}} \text{ is the } i\text{th component of the gradient operator;} \\ L^{(j)} &:= b^{(j)\top} \nabla \text{ is a scalar operator;} \\ c^{(j_1 j_2)}(x, t) &:= L^{(j_1)} b^{(j_2)}(x, t) : \mathbb{R}^l \times \mathcal{T} \rightarrow \mathbb{R}^l \\ \bar{f}(x_n, t_n) &:= f(x_n, t_n)h + B(x_n, t_n)\Delta W_n + \sum_{j_1=1}^m \sum_{j_2=1}^m c^{(j_1 j_2)_n}(x_n, t_n) I_{(j_1 j_2)} \\ \bar{f}_n &:= \bar{f}(x_n, t_n); \quad f_n := f(x_n, t_n); \quad B_n := B(x_n, t_n); \quad c_n^{(j_1 j_2)} := c^{(j_1 j_2)}(x_n, t_n) \\ \Delta f_n &:= f_{n+1} - f_n; \quad \Delta B_n := B_{n+1} - B_n; \quad \Delta c_n^{(j_1 j_2)} := c_{n+1}^{(j_1 j_2)} - c_n^{(j_1 j_2)} \\ \Delta \phi_n &:= \Delta f_n h + \sum_{j_1=1}^m \sum_{j_2=1}^m \Delta c_n^{(j_1 j_2)} I_{(j_1 j_2)_n}. \end{aligned} \quad (4.1)$$

Then the FIS- α numerical scheme is given as

$$x_{n+1} = x_n + \bar{f}_n + \frac{\beta}{\gamma} \alpha \mathcal{P}_n \Delta \phi_n + \left(\frac{1}{2} - \frac{\beta}{\gamma} \right) a_n \quad (4.2)$$

$$a_{n+1} = \frac{1}{\gamma} \Delta \phi_n + \left(1 - \frac{1}{\gamma} \right) a_n \quad (4.3)$$

where $\infty \gg \alpha > 1$ is a user-selectable real parameter; \mathcal{P}_n is a real weight matrix \mathcal{P} at the n th time step having $\|\mathcal{P}_n\| = 1$ with probability 1 such that the real part of the eigenvalues of $\mathcal{I} - \frac{\beta}{\gamma} \alpha \mathcal{P}_n \left(\frac{\partial}{\partial x} (fh + \sum_{j_1=1}^m \sum_{j_2=1}^m \Delta c^{(j_1 j_2)} I_{(j_1 j_2)_n}) \right)_{x=x}$ (\mathcal{I} being the identity matrix and the derivative term is evaluated at x which is an iterate in computing the n th time step) is always non-negative, and

$$\gamma = \frac{2}{\rho + 1} - \frac{1}{2} \quad (4.4)$$

$$\beta = \frac{1}{(\rho + 1)^2} \quad (4.5)$$

$$a_0 = h^2 \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} f \right)_{t=t_0, x=x_0} =: h^2 k_0 < \infty \text{ almost surely.} \quad (4.6)$$

The parameter $\rho \in [0, 1) \subset \mathbb{R}$ is also user-selectable. The construction of γ and β are explained in [21]. Since f is assumed to be linear growth bounded (assumption A4) along with $\|x_0\| < \infty$ with probability 1 (assumption A5), we have a_0 to be finite almost surely. The recurrence (4.3) can be expanded as

$$a_n = \left(1 - \frac{1}{\gamma} \right)^n a_0 + \frac{1}{\gamma} \sum_{j=1}^n \left(1 - \frac{1}{\gamma} \right)^{j-1} \Delta \phi_{n-j} \quad (4.7)$$

indicating that a feeds back the response from past time steps to affect in both drift and diffusion the numerical damping that helps in simulation of stiff systems.

4.1. Computation of \mathcal{P}_n

There are several ways to compute the weight matrix \mathcal{P}_n which is similar to that in the balanced implicit and balanced Milstein methods [19,13,32]. For definiteness, we use the following way to compute \mathcal{P}_n in this work. The real Schur decomposition of the Jacobian $\mathcal{J}_i := \left(\frac{\partial}{\partial x} \left(fh + \sum_{j_1=1}^m \sum_{j_2=1}^m c^{(j_1 j_2)} I_{(j_1 j_2)_n} \right) \right)_{x=x_i}$ (i.e., the Jacobian \mathcal{J} evaluated at some iterate x_i in the Newton iteration for computing x at the mesh point t_{n+1}) is used for computing \mathcal{P}_n . Let $\mathcal{J}_i = Q_i T_i Q_i^T$ be the real Schur decomposition where Q is a unitary matrix and T_i is an upper Hessenberg matrix with 1×1 and 2×2 diagonal blocks corresponding to the real and complex eigenvalues of \mathcal{J}_i , respectively. We can then compute \mathcal{P}_n corresponding to the iterate x_i as $Q_i \tilde{T}_i Q_i^T$ where \tilde{T}_i is a diagonal matrix with the entry of -1 if the corresponding diagonal entry of T_i is positive. The diagonal entry in \tilde{T}_i is 1 if the corresponding diagonal entry of T_i is zero or negative. It may be noted that by this construction $\|\mathcal{P}\|_2 = 1$ with probability 1 for all time steps and for any iterate.

4.2. Mean-square estimation of $\Delta\phi_n$

Lemma 4.1. *With h being the time step size on a uniform mesh and $\Delta\phi$ defined as in (4.1), we have $E(\Delta\phi_n)^2 | \mathcal{A}_{t_n} \leq Kh^3$ where K is a suitable constant independent of h and $\mathcal{A}_{t_n}, t_n > t_0$ is the sub- σ algebra as defined in assumption A2.*

Proof. For any deterministic function $\zeta(x, t)$ representing a component of f, B or $c^{(j_1 j_2)}$, we write the Itô-Taylor expansion

$$\Delta\zeta = \underbrace{\left(\frac{\partial\zeta}{\partial t} + f^T \nabla\zeta + \frac{1}{2} \text{trace}(BB^T \nabla[\nabla\zeta]) \right)_{x=x_n, t=t_n}}_{\zeta_{D_n}} h + \underbrace{(\nabla\zeta^T B)_{x=x_n, t=t_n}}_{\zeta_{M_n}} \Delta W_n + O(h) \tag{4.8}$$

with a root mean square estimate of the remainder terms. By assumption A4 each of the coefficient terms in the above expansion, e.g., ζ_{D_n}, ζ_{M_n} is linear growth bounded. Applying (4.8) to the components of f, B and $c^{(j_1 j_2)}$ as necessary, we can have the following expansion.

$$\Delta\phi_n = f_{D_n} h^2 + f_{M_n} \Delta W_n h + \sum_{j_1=1}^m \sum_{j_2=1}^m \left(c_{D_n}^{(j_1 j_2)} h I_{(j_1 j_2)_n} + c_{M_n}^{(j_1 j_2)} \Delta W_n I_{(j_1 j_2)_n} \right) + \dots \tag{4.9}$$

where $f_{M_n}, c_{M_n}^{(j_1 j_2)}$ are matrices and $f_{D_n}, c_{D_n}^{(j_1 j_2)}$ are column vectors. In (4.9) it may be noted that $f_{M_n} \Delta W_n h$ produces the largest root mean square term, i.e., of $O(h^{\frac{3}{2}})$. Then, we can estimate the following expectation:

$$\mathbf{E} \left(\sup_{[t_n, t_{n+1}]} \|\Delta\phi_n\|^2 | \mathcal{A}_{t_n} \right) \leq (K_1 + K_2 \|x_n\|^2) h^3 \tag{4.10}$$

where the K 's are suitable constants. Similarly, we obtain

$$\mathbf{E} \left(\sup_{[t_n, t_{n+1}]} \Delta\phi_{k_1}^T \Delta\phi_{k_2} | \mathcal{A}_{t_{k_1}}, \mathcal{A}_{t_{k_2}} \right) \leq (K_3 + K_4 \|x_{k_1}\|^2 + K_5 \|x_{k_2}\|^2) h^4 \tag{4.11}$$

for any $k_1 \neq k_2, k_1, k_2 \in \{1, \dots, N\}$ by using the assumptions A4 and A6, since the Wiener increments are independent across the time steps.

From the above analysis we can conclude that $\Delta\phi$ is an $O(h^3)$ term in the mean square sense. \square

5. Strong order of the FIS- α approximation

In this section we establish the strong order (as defined in [15]) of the accuracy of the approximation made by the FIS- α method. Wherever necessary we assume Lipschitz continuity and linear growth bound as stated in the assumptions A3 and A4. The K 's used in the following analysis are suitable finite constants independent of the fixed time step size h .

Theorem 5.1. *The FIS- α method as in (4.2) and (4.3) has a strong order 1.0 of consistency.*

Proof. We observe that $x_n + \bar{f}_n$ in (4.2) is the Milstein scheme [18,20] and has a local strong order of approximation of 1.0 under the assumptions A1–A5 (cf. Theorem 10.3.5 in [15]). The following estimate then holds (see Chapter 10, [15]).

$$\mathbf{E} \left(\sup_{[t_n, t_{n+1}]} \left\| \int_{t_n}^{t_{n+1}} f(x_s, s) ds + \int_{t_n}^{t_{n+1}} B(x_s, s) dW_s - \bar{f}_n \right\|^2 | \mathcal{A}_{t_n} \right) \leq (K_6 + K_7 \|x_n\|^2) h^3. \tag{5.1}$$

where x_s denotes x at $t = s$ and $\mathcal{A}_{t_i}, t_i > t_0, i = 1, \dots, n, n + 1, \dots, N$ is the sub- σ algebra as defined in assumption A2. Then, using the estimates (4.10) and (4.11) (as established in Lemma 4.1) for the expansion (4.7) we can write the following.

$$\begin{aligned} & \mathbf{E} \left(\max_{\{t_0, \dots, t_n\}} \left| \frac{1-\beta}{2} - \frac{\beta}{\gamma} \right|^2 \|a_n\|^2 | \mathcal{A}_{t_n}, \dots, \mathcal{A}_{t_0} \right) \\ & \leq 2 \left| \frac{1-\beta}{2} - \frac{\beta}{\gamma} \right|^2 \left(\frac{\left| \frac{1}{\gamma} \right|^2}{1 - \left| 1 - \frac{1}{\gamma} \right|^2} \left(1 - \left| 1 - \frac{1}{\gamma} \right|^{2n} \right) \left(K_8 + K_9 \max_{l \in \{0, \dots, n\}} \|x_l\|^2 \right) h^3 + 2 \left| 1 - \frac{1}{\gamma} \right|^{2n} k_0^2 h^4 \right) + O(h^4) \leq \left(K_{10} + K_{11} \max_{l \in \{0, \dots, n\}} \|x_l\|^2 \right) h^3. \end{aligned} \tag{5.2}$$

since $|1 - \frac{1}{\gamma}| < 1$, $0 \leq \left| \frac{1}{2} - \frac{\beta}{\gamma} \right| \frac{\left| \frac{1}{\gamma} \right|^2}{1 - \left| 1 - \frac{1}{\gamma} \right|^2} \leq \frac{1}{6}$, $0 \leq \left| \frac{1}{2} - \frac{\beta}{\gamma} \right|^2 \frac{\left| \frac{1}{\gamma} \right|^2}{1 - \left| 1 - \frac{1}{\gamma} \right|^2} \leq 0.014$ and $\frac{1}{2} \leq \left| \frac{1}{2} - \frac{\beta}{\gamma} \right| \leq \frac{2}{3}$ for $\rho \in [0, 1)$. The estimates 4.10, 5.1 and 5.2 together lead to the local strong order of convergence of the scheme (4.2) and (4.3) as follows:

$$\begin{aligned} & \mathbf{E} \left(\sup_{\{t_n, t_{n+1}\}} 2 \left\| \int_{t_n}^{t_{n+1}} f(x_s, s) ds + \int_{t_n}^{t_{n+1}} B(x_s, s) dW_s - \bar{f}_n \right\|^2 + 4 \|\mathcal{P}_n\|^2 \alpha^2 \left| \frac{\beta}{\gamma} \right|^2 \|\Delta\phi_n\|^2 + 4 \left| \frac{1-\beta}{2} - \frac{\beta}{\gamma} \right|^2 \|a_n\|^2 | \mathcal{A}_{t_n} \right) \\ & \leq \mathbf{E} \left(\sup_{\{t_n, t_{n+1}\}} 2 \left\| \int_{t_n}^{t_{n+1}} f(x_s, s) ds + \int_{t_n}^{t_{n+1}} B(x_s, s) dW_s - \bar{f}_n \right\|^2 | \mathcal{A}_{t_n} \right) + 4 \mathbf{E} \left(\sup_{\{t_n, t_{n+1}\}} \|\mathcal{P}_n\|^2 \alpha^2 \left| \frac{\beta}{\gamma} \right|^2 \|\Delta\phi_n\|^2 | \mathcal{A}_{t_n} \right) \\ & \quad + 4 \mathbf{E} \left(\max_{\{t_0, \dots, t_n\}} \left| \frac{1-\beta}{2} - \frac{\beta}{\gamma} \right|^2 \|a_n\|^2 | \mathcal{A}_{t_n}, \dots, \mathcal{A}_{t_0} \right) \\ & \leq \left(K_{12} + K_{13} \|x_n\|^2 + K_{14} \max_{l \in \{0, \dots, n\}} \|x_l\|^2 \right) h^3. \end{aligned} \tag{5.3}$$

Thus the FIS- α method can be considered as a Milstein scheme plus some additional terms that do not change the order of the mean-square error of the Milstein scheme. Applying Theorem 10.8.3 in [15] to the local mean-square error estimate (5.3) of the FIS- α method, the strong order consistency of the FIS- α is then established as 1.0, i.e.,

$$\begin{aligned} & \mathbf{E} \left(\sup_{\{t_0, t_f\}} \left\| \int_{t_0}^{t_f} f(x_s, s) ds + \int_{t_0}^{t_f} B(x_s, s) dW_s - x_{N-1} - x_0 - \bar{f}_{N-1} - \frac{\beta}{\gamma} \alpha \mathcal{P}_{N-1} \Delta\phi_{N-1} - \left(\frac{1-\beta}{2} - \frac{\beta}{\gamma} \right) a_{N-1} \right\|^2 | \mathcal{A}_{t_0} \right) \\ & \leq (K_{15} + K_{16} \|x_0\|^2) h^3. \quad \square \end{aligned} \tag{5.4}$$

5.1. Positivity preserving conditions

When an SDE needs pathwise preservation of positivity, the application will be restricted by the following condition on the FIS- α method.

From (4.2) a positivity preserving condition for the FIS- α method can be seen to be

$$\bar{f}_n + \frac{\beta}{\gamma} \alpha \mathcal{P}_n \Delta\phi_n + \left(\frac{1-\beta}{2} - \frac{\beta}{\gamma} \right) a_n > 0 \tag{5.5}$$

for eternal life time of the method, i.e., for obtaining $P(x_{n+1} > 0 | x_n > 0) = 1$. It may be noted that $\frac{\beta}{\gamma} \alpha \mathcal{P}_n \Delta\phi_n$ can be effectively taken as non-negative using the construction of \mathcal{P}_n and non-negativity of $\frac{\beta}{\gamma}$. Then the condition

$$\bar{f}_n + \left(\frac{1-\beta}{2} - \frac{\beta}{\gamma} \right) a_n > 0 \tag{5.6}$$

needs to be satisfied for eternal life of the FIS- α method. It is easy to see that the condition (5.6) has a global minimum in case of diagonal noise if each $c_n^{(j,j)}$, $j \in \{1, \dots, m\}$ is non-negative and then the positivity preserving conditions can be obtained similar to that for the Balanced Milstein Method in [13]. Since our main objective is to study the stiffness in diffusion, we do not elaborate on this property further in the present study.

6. Mean square stability of the FIS- α method

Following the established practice [12,3,4,24,25,23] for analyzing the stochastic stability of a numerical integrator in the mean square sense, we take a one-dimensional linear test SDE with a single channel of noise:

$$dx = \bar{\lambda} x dt + \bar{\eta} x dW_t \tag{6.1}$$

for our stability analysis and define

$$\chi := \bar{\lambda}h + \bar{\eta}^2 \frac{\left(\int_0^h dW_s\right)^2 - h}{2} := \bar{\lambda}h + \bar{\eta}^2 h \frac{\xi^2 - 1}{2} := \lambda + \eta^2 \frac{\xi^2 - 1}{2}, \quad \lambda := \bar{\lambda}h, \eta := \bar{\eta}\sqrt{h}; \xi \sim N(0, 1) \text{ i.e., } \xi \text{ is Gaussian distributed with zero mean and unit variance.} \quad (6.2)$$

As per the construction in the Section 4.1, we set \mathcal{P}_η for the discretization (4.2) of the one-dimensional single channel noise test Eq. (6.1) to be a scalar p such that $\Re\left(1 - \frac{\beta}{\gamma}\alpha\mathcal{P}_\eta\chi\right) = \Re\left(1 - \frac{\beta}{\gamma}\alpha p\chi\right) > 0$ for all values of $\chi \in \mathbb{C}$. The construction in the Section 4.1 leads us to compute $p = \exp(i(\pi - 2\arg(\chi)))$, $i = \sqrt{-1}$ if $\chi \in \mathbb{C}^+$ and $p = 1$ otherwise. The discretization (4.2) and (4.3) of (6.1) then yields the amplification matrix for the FIS- α method as follows:

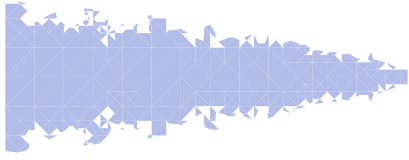
$$A := \begin{pmatrix} \frac{\chi\gamma}{\gamma - \beta\alpha p\chi} + 1 + \gamma \frac{\eta\xi}{\gamma - \beta\alpha p\chi} & \frac{\gamma - 2\beta}{2(\gamma - \beta\alpha p\chi)} \\ \frac{\chi^2 + \chi\eta\xi}{\gamma - \beta\alpha p\chi} & \left(1 - \frac{1}{\gamma}\right) + \frac{\frac{1}{2}\frac{\beta}{\gamma}}{\gamma - \beta\alpha p\chi} \end{pmatrix} \quad (6.3)$$

so that $(x_{n+1}a_{n+1})^\top = A(x_n a_n)^\top$ along a given sample path. The maximum magnitude of the eigenvalues of A determines the contractivity of the map $(x_{n+1}, a_{n+1}) \leftarrow (x_n, a_n)$ (cf. Chapter IV.11 in [10]) along a given sample path. The maximum magnitude of the eigenvalues of A is given by

$$\begin{aligned} R(\lambda, \eta, \xi) := & \max\left(\left|(2(\chi + \eta\xi + 2)\gamma^2 + (4\alpha\beta\text{sign}(\chi)\chi + \chi - 2)\gamma - 2\beta\chi(\alpha\text{sign}(\chi) + 1)\right.\right. \\ & \left.\left. + \left((-2\beta\chi + 2\alpha\beta(2\gamma - 1)\text{sign}(\chi)\chi + \gamma(2\gamma\chi + \chi + 2\gamma(\eta\xi + 2) - 2)\right)^2\right.\right. \\ & \left.\left. - 8\gamma(\gamma + \alpha\beta\chi\text{sign}(\chi))(-2\beta\chi + 2\alpha\beta(\gamma - 1)\text{sign}(\chi)\chi + \gamma(\chi(2\gamma - 1)\right.\right. \\ & \left.\left. + 2(\gamma - 1)(\eta\xi + 1))\right)^{1/2}\right)/(4\gamma(\gamma + \alpha\beta\chi\text{sign}(\chi))) \end{aligned} \quad (6.4)$$

for $\lambda \in \mathbb{R}$ and $\eta \in \mathbb{R}$. From the structure of $R(\lambda, \eta, \xi)$ in (6.4) it can be seen that \mathcal{P}_η in the formulation (4.2) and (4.3) as constructed in Section 4.1 removes any singularity from $R(\lambda, \eta, \xi)$ and admits it as a proper integrand (to (6.5)) for defining the mean square stability of the FIS- α method. Following [12,3,4,6,32,1], the mean square stability region of an SDE integrator is defined over the $(\lambda \in \mathbb{R}^-, \eta \in \mathbb{R})$ plane. This leads to the following definition.

Definition 6.1. For a given $\rho \in [0, 1)$ and a given $1 <$



1. We choose a $\rho \in [0.0, 0.8]$, an $\alpha \in [4.0, 8.0]$ and a time step size h according to the accuracy requirement.
2. From the generated random numbers for the simulation of the Wiener process we compute the Itô integrals. The double Itô integrals may be computed as approximated in Chapter 5 of [15] with sufficiently large number of terms.
3. The SDE to be integrated is discretized with (4.2) and (4.3).
4. For use in Newton iterations we first compute the real Schur decomposition of the Jacobian $\left(\frac{\partial}{\partial x} \left(fh + \sum_{j_1=1}^m \sum_{j_2=1}^m c^{(j_1, j_2)} I_{(j_1, j_2)_n} \right)\right)_{x=x_n}$. Using this real Schur decomposition, \mathcal{P}_n is computed as described in Section 4.1. Whenever the Jacobian is updated in the Newton iterations, \mathcal{P}_n is re-computed at an intermediate Newton iterate x_i using the real Schur decomposition of $\left(\frac{\partial}{\partial x} \left(fh + \sum_{j_1=1}^m \sum_{j_2=1}^m c^{(j_1, j_2)} I_{(j_1, j_2)_n} \right)\right)_{x=x_i}$. The real Schur decomposition is re-used for the solution of the linear system in the Newton Iteration. It may be mentioned that in our implementation of the method we use the Matlab™ automatic differentiation tool myAD (<http://www.mathworks.com/matlabcentral/fileexchange/15235>) (see www.autodiff.org for various other automatic differentiation tools) or a symbolic computer algebra system like the Mathematica™ to generate the derivative $\frac{\partial}{\partial x} \left(fh + \sum_{j_1=1}^m \sum_{j_2=1}^m c^{(j_1, j_2)} I_{(j_1, j_2)_n} \right)$ which is then evaluated at an iterate x_i followed by its real Schur decomposition. This approach tends to give faster convergence and to need less frequent Jacobian updates in the Newton iterations.
5. x for the $n + 1$ th mesh point is computed when the Newton iterations converge to a given tolerance.
6. On Newton convergence, a is updated as (4.3).

7.1. Remark: a two-step method

The discretization (4.2) and (4.3) can be written as a balanced implicit two-step method

$$x_{n+1} - \left(2 - \frac{1}{\gamma}\right)x_n + \left(1 - \frac{1}{\gamma}\right)x_{n-1} = \bar{f}_n - \left(1 - \frac{1}{\gamma}\right)\bar{f}_{n-1} + \frac{\beta}{\gamma}\alpha\mathcal{P}_n\Delta\phi_n + \left(\frac{1}{2} - \frac{\beta}{\gamma}\right)\left(\frac{1}{\gamma} - \left(1 - \frac{1}{\gamma}\right)\frac{\beta}{\gamma}\alpha\right)\Delta\phi_{n-1} \tag{7.1}$$

by using the expression for a_n as given by the recurrence (4.3) and by eliminating a_{n-1} . The scheme has the same mean-square error and stability properties as the FIS- α method, since each of the steps are FIS- α method steps and has the same mean-square error and same stability properties of the FIS- α method. In the two-step scheme (7.1), \mathcal{P}_n is computed in the same way as in Section 4.1 as a matrix transformation which reflects the eigenvalues of the operand matrix on the right half complex plane to the left half plane. When computing $\mathcal{P}_n\Delta\phi_n$, the real Schur decomposition of $\left(\frac{\partial}{\partial x} \left(fh + \sum_{j_1=1}^m \sum_{j_2=1}^m c^{(j_1, j_2)} I_{(j_1, j_2)_n} \right)\right)_{x=x_i}$ at some Newton iterate x_i toward the solution of x_{n+1} is used. In our simulations in the next section we, however, use the one step method (4.2) and (4.3).

8. Numerical examples

In this section, we give some numerical examples that demonstrate the computational efficiency, the convergence properties and the stability of the FIS- α method.

8.1. Linear examples

The following linear examples are used to validate the strong convergence and stability property of the FIS- α method against known analytical solutions.

8.1.1. Linear Example 1

We consider the stiff SDE:

$$dx_t = Ux_t dt + Vx_t dW_t, \quad x(t_0) = x_0, \quad t \in [0, 1], \quad x \in \mathbb{R}^2, \tag{8.1}$$

where $U := \begin{pmatrix} -u & u \\ u & -u \end{pmatrix}$ and $V := \begin{pmatrix} v & 0 \\ 0 & v \end{pmatrix}$. The exact solution [15] of this equation is given by

$$x_t = T \begin{pmatrix} \exp(\rho^+(t)) & 0 \\ 0 & \exp(\rho^-(t)) \end{pmatrix} T^{-1} x_0,$$

where $T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, $\rho^\pm(t) = (-u - \frac{1}{2}v^2 \pm u)t + vW(t)$, $x_0 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ almost surely and $T = T^{-1}$. This equation is stiff in both its deterministic and stochastic components (u and v , respectively). With a drift implicit scheme a correct numerical solution can be obtained only for very small step sizes [30,6] and hence a fully implicit scheme is necessary to integrate it. For our computations we take $u = 5$, $v = 10$ and the initial value $x_0 = (1 \ 2)^T$ as given in [15]. The error plots in the Figs. 8.1–8.3 establish the stability and error behavior of the FIS- α method consistent with Figs. 6.2 and 6.3 and Theorem 5.1, respectively.

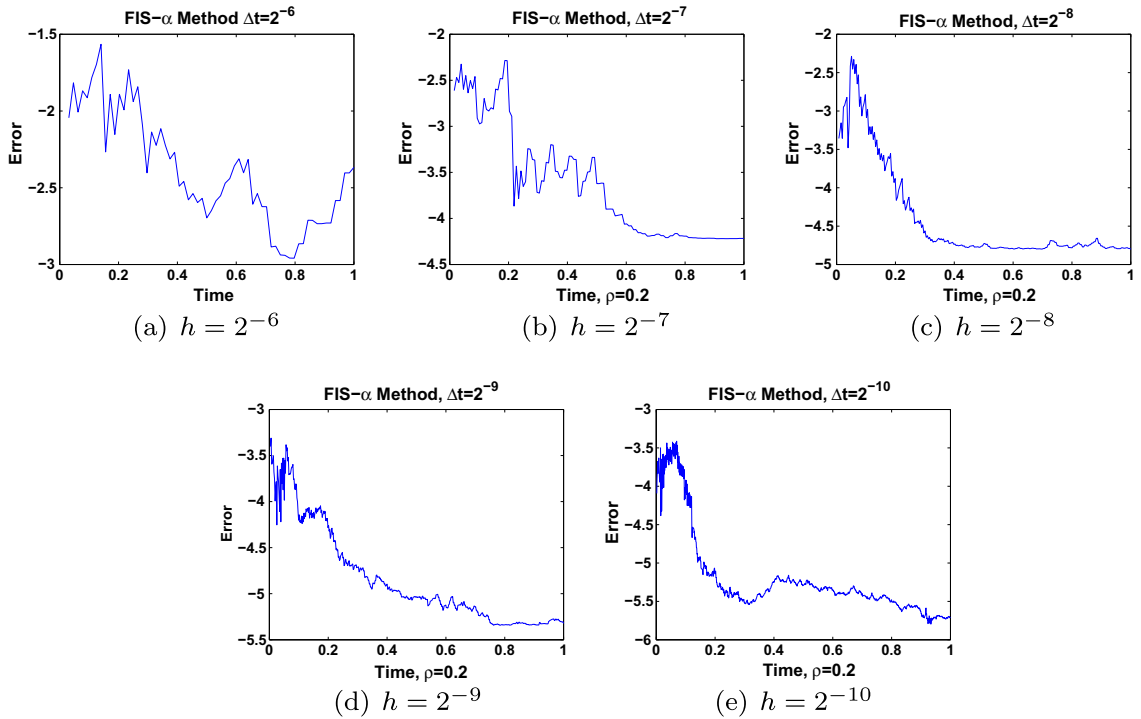


Fig. 8.1. \log_{10} of the arithmetic average of the 2-norm of the error in x in integrating (8.1) (with $u = 5, v = 10$) by the FIS- α method over 1500 independent sample paths using various values of time step sizes h and $\rho = 0.2, \alpha = 8$.

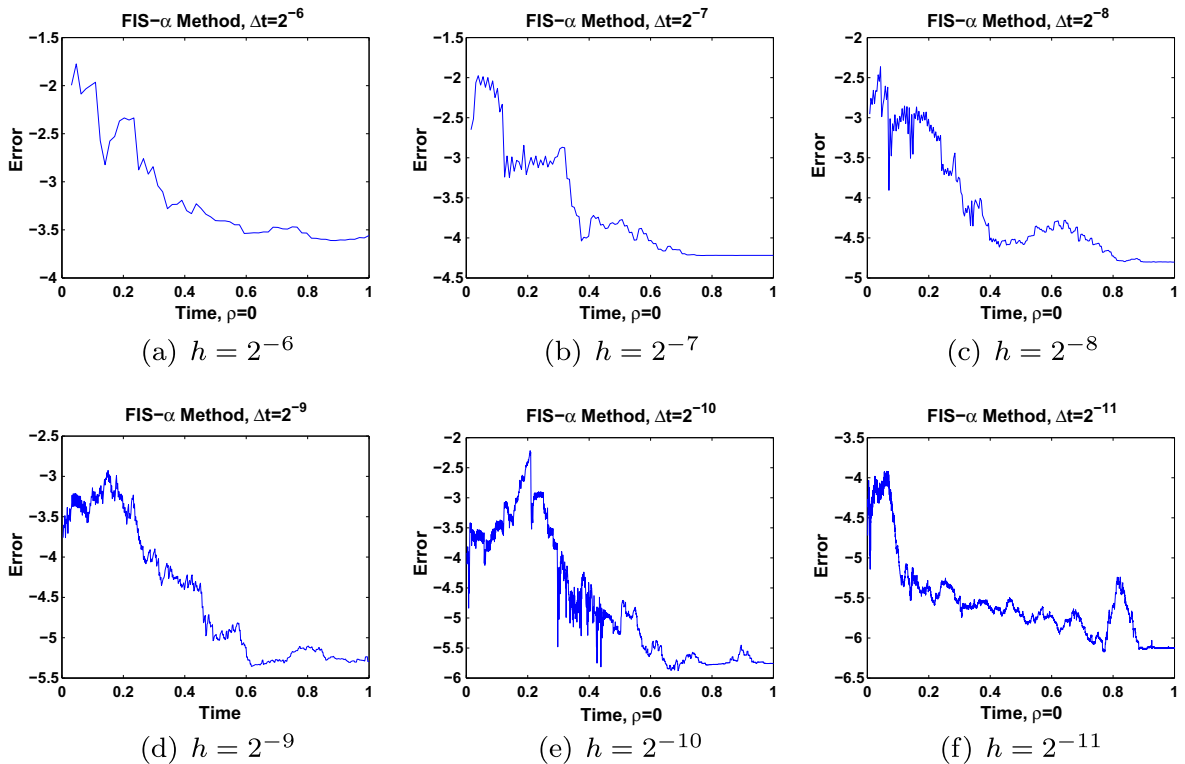


Fig. 8.2. \log_{10} of the arithmetic average of the 2-norm of the error in x in integrating (8.1) (with $u = 5, v = 10$) by the FIS- α method over 1500 independent sample paths using various values of time step sizes h and $\rho = 0, \alpha = 4$.

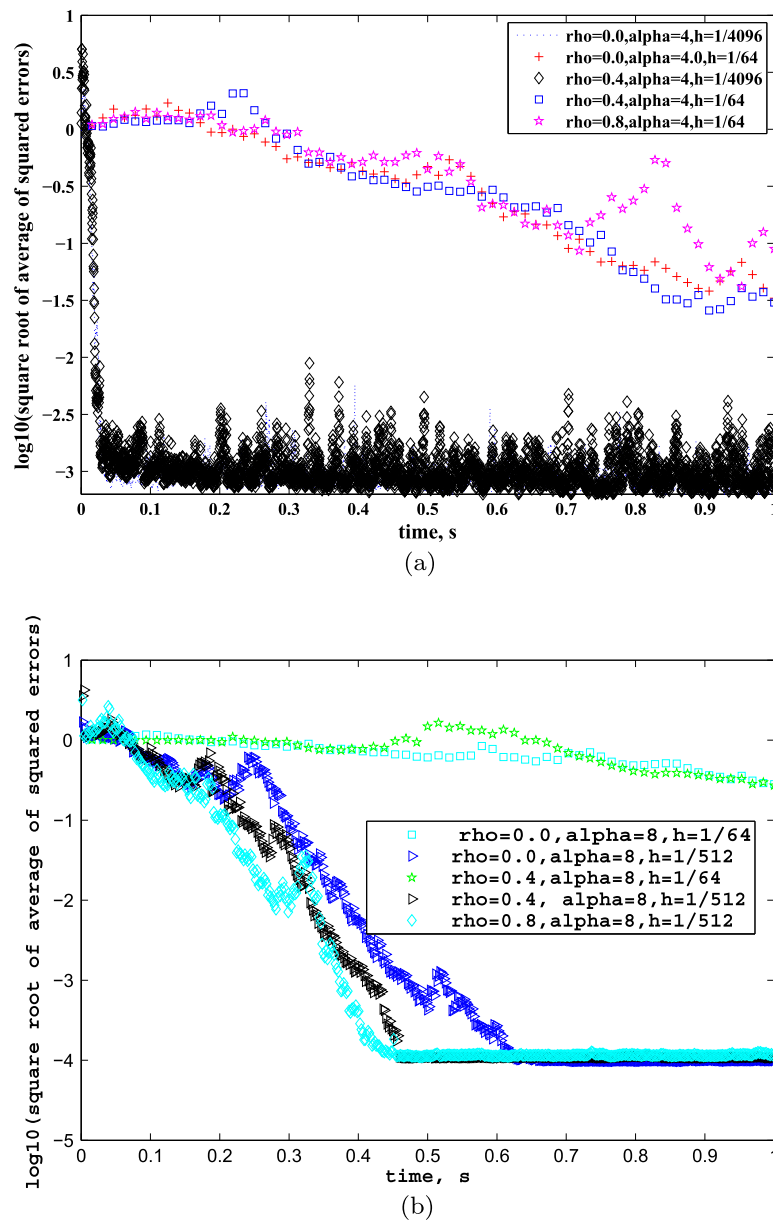


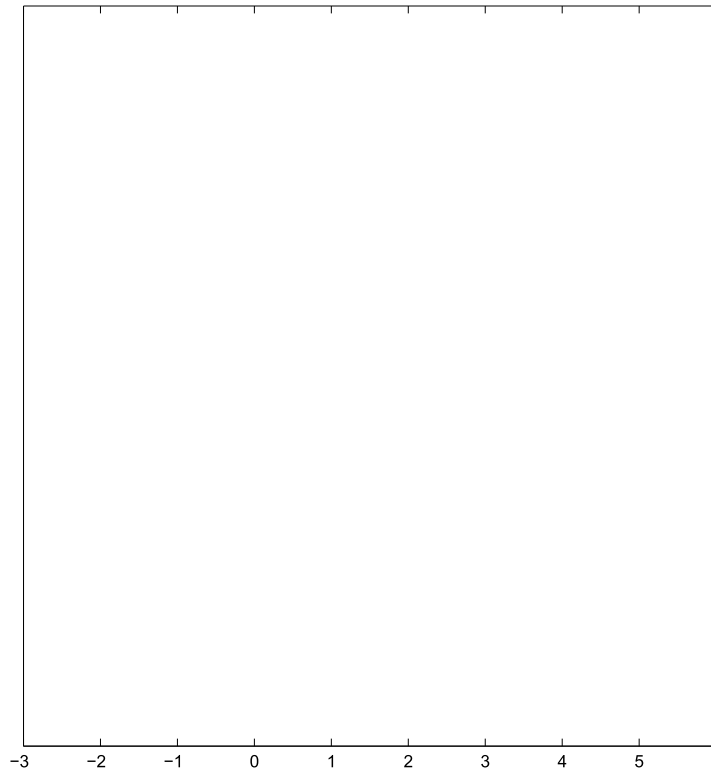
Fig. 8.4. \log_{10} of the arithmetic average of the errors squared in x in integrating (8.2) by the FIS- α method over 1500 independent sample paths for each case. The stabilization of the error and convergence of the numerical solution even with the relatively larger time step sizes of 2^{-6} and 2^{-9} demonstrate the efficiency of the FIS- α method.

with $x_{t_0} = (26)^T$ almost surely. The normalized simulation interval is taken as $[0.0, 1.0]$. The diffusion coefficient on the first noise channel is multiplicative but the second channel is additive. This makes the noise in (8.4) commutative. The coefficients for the double Itô integrals $\int_0^h \int_{i \neq j, i, j=1,2} W_s^{(i)} dW_s^{(j)}$ become zero in the FIS- α method resulting in fewer computations.

In [26] it has been shown that (8.3) and (8.4) is forward complete. This stable non-explosion behavior is shown in Fig. 8.5 obtained by integrating (8.3) and (8.4) with the FIS- α method over 1500 independent sample paths for each of the various combinations of values of ρ , α and h . Each of the sample paths is realized with a tolerance of 10^{-6} for the Newton iterations.

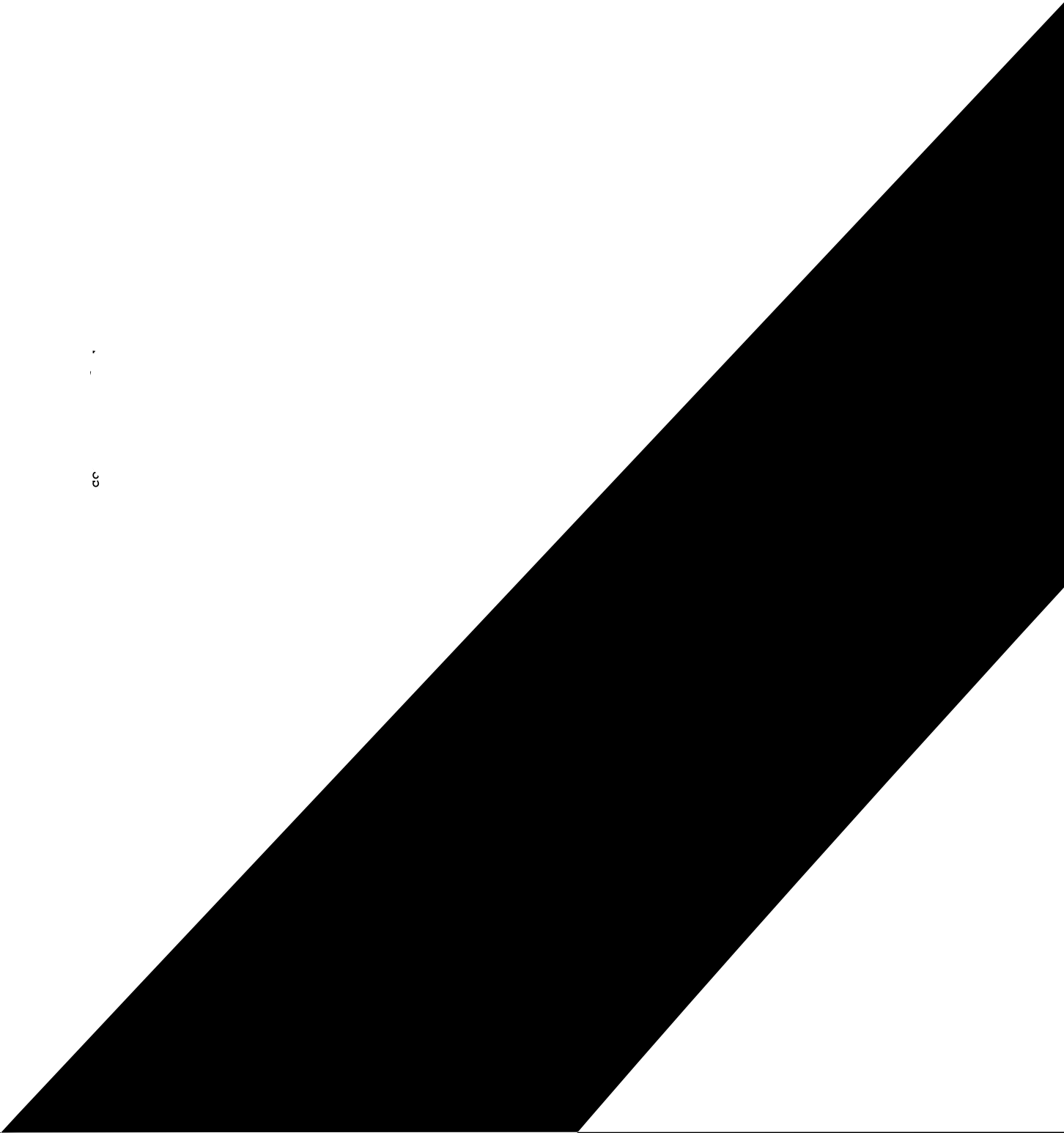
8.3. Chemical Langevin equation

When in a well stirred finite volume v a finite number l of distinct chemical species having the states $x^{(i)} > \epsilon |v_{j,i}|$, $i = 1, \dots, l, j = 1, \dots, m, \mathbb{R} \ni \epsilon > 0$ (v being the stoichiometric matrix with $v_{j,i}$ as the entry for the i th species participating in the j th reaction) participate in m chemical reactions with the propensities $\varphi^{(j)}(x, t) > \delta \gg 1, j = 1, \dots, m$; the chemical



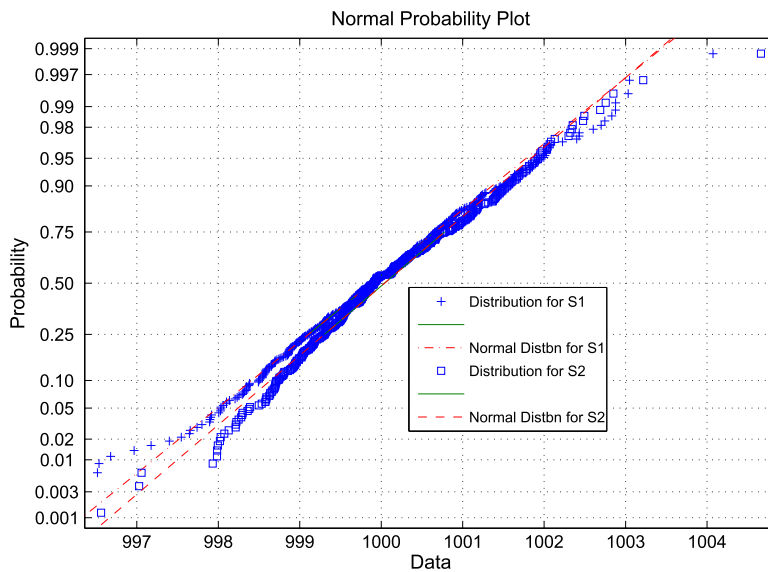
reactions along with the uncertainties in the kinetics can be modeled as a system of chemical Langevin equations (CLEs) [29,31]. Assuming that the approximations allowed in the thermodynamic limit hold [29,31], the model of the chemical reactions is given by the following system of CLEs.



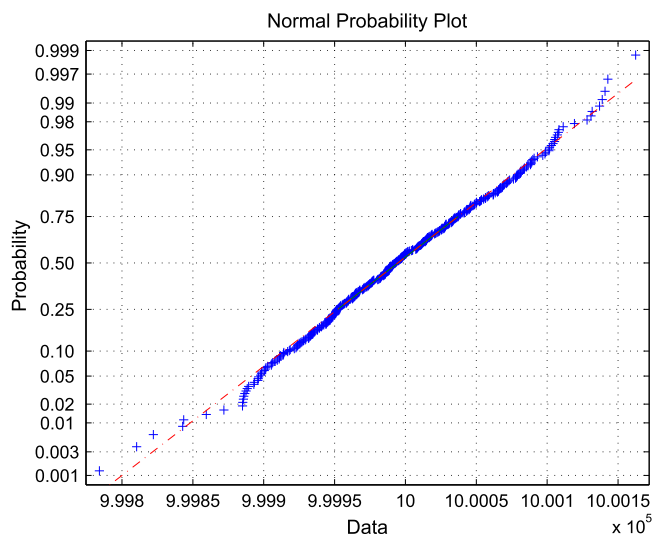


The following points when compared with [29] demonstrate the computational efficiency of the FIS- α method.

- Larger time steps: Compared to the adaptive time step scheme in [29] the FIS- α method can take larger (2^{-8} for FIS- α method compared to 10^{-4} in [29]) time steps. We have been able to take step size as large as 2^{-6} with a Newton iteration tolerance of 10^{-6} . Also, the FIS- α method is able to simulate the CLEs for 10 times longer time interval compared to that in [29].
- Computational effort: For the CLEs of (8.6) the average computational effort a single time step for our implementation is about 2.5 times the explicit Milstein scheme (which is not very effective against stiffness and cannot integrate the CLEs of (8.6) with time steps larger than 5×10^{-7}) and about the same as the balanced implicit Milstein scheme in [32]. However, the ability to take much larger time steps gives the present method its computational efficiency.
- Speed-up over [29]: On a Sun Fire X2200 M2™ Server with 2 Quad-Core AMD Opteron™ Model 2356, 2.3 GHz processors along with 32 GB memory, the method described in [29] was benchmarked for the CLEs for the reaction system (8.6) with a mean CPU time of 23.78 s per realization over the interval of [0.0, 0.1], the average being taken over 10,000



(a) Probability plot for S_1, S_2 against Gaussian probability (straight lines)



(b) Probability plot for S_3 against Gaussian probability (straight line)

Fig. 8.8. Chemical Langevin equations: probabilities of the states of the species at $t = 0.05$ against Gaussian probability plots for each species obtained with 2500 independent sample path realizations.

realizations. The Matlab™ implementation used up to 8 threads and a Newton tolerance of 10^{-6} . Using same tolerance and similar threaded Matlab™ implementation on the same machine, the FIS- α method simulation takes a maximum of 4.23 CPU seconds for one realization when using the smallest time step size of 1/1024. It may be noted that 2500 realizations were sufficient for a weak convergence (discussed below) of the computations. The CPU times must be taken as indicative since the absolute numbers can vary with the state and configuration of the operating system.

- (d) Smaller variance: The Fig. 8.6(a)–(c) show that the spread of the mean state of the species over the simulation interval is of the order of 0.003% about the theoretical mean compared to the 0.05% spread in [29]. The coefficients of variation in Fig. 8.7(a)–(c) are also quite small and thus show that the FIS- α method has a small variance with respect to the simulation of the CLEs of (8.6).
- (e) Convergence in distribution: The distribution of each species (the states being stationary processes) at a given time point is expected to be a Gaussian distribution for (8.6) [29]. In the Fig. 8.8(a) and (b) the dotted straight lines represent the Gaussian distribution against which the data for the 3 species at midpoint of the simulation interval is plotted. The convergence in distribution is readily seen. It may be pointed out that this weak convergence is comparable to that in [29] and is obtained with only 2500 realizations of independent sample paths as against 10,000 in [29]. This reduced computational effort demonstrates the reduced variance of the present method for the CLE problem.

Remark. It may be mentioned that the speed-up of the FIS- α method over adaptive time stepping Milstein scheme (which is an explicit method and does not need Newton iterations) discussed above does not scale uniformly for a any given problem. It is strongly related to the number of iterations needed for Newton convergence in each time step of a realization of a given sample path. A tighter tolerance induces typically more Newton iterations and the FIS- α slows down. For the present problem we needed an average of 4 iterations per time step in the `fsolve` routine of Matlab™ under the tolerance of 10^{-6} . A tolerance of 10^{-3} reduces this to 2 iterations while tightening it to 10^{-12} induces 11 iterations. The above speed-up and iterations numbers must be taken only as indicative and we observe that faster algorithms and more sophisticated implementations of Newton iteration schemes can vary the above numbers quite differently.

9. Conclusion

In this work we have constructed and implemented a fully and balanced implicit Milstein scheme which has a very large stability region and thus addresses the stability region deficiency pointed out in [16]. Computational experiments demonstrate that the present method efficiently simulates problems that have significant stiffness in the diffusion coefficients. In particular, a CLE system which is driven by stiff noise is shown to be efficiently simulated by the FIS- α method.

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