Magnus Exponential Integrators for Stiff Time-Varying Stochastic Systems

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We introduce exponential numerical integration methods for stiff stochastic dynamical systems of the form $d\mathbf{z}_t = L(t)\mathbf{z}_t dt + \mathbf{f}(t)dt + Q(t)d\mathbf{W}_t$. We consider the setting of time-varying operators $L(t), Q(t)$ where they may not commute $L(t_1)L(t_2) \neq L(t_2)L(t_1)$, raising challenges for exponentiation. We develop stochastic numerical integration methods using Mangus expansions for preserving statistical structures and for maintaining fluctuation-dissipation balance for physical systems. For computing the contributions of the fluctuation terms, our methods provide alternative approaches without needing directly to evaluate stochastic integrals. We present results for our methods for a class of SDEs arising in particle simulations and for SPDEs for fluctuations of concentration fields in spatially-extended systems. For time-varying stochastic dynamical systems, our introduced discretization approaches provide general exponential numerical integrators for preserving statistical structures while handling stiffness.

1 Introduction

Stochastic modeling is used in many areas of the sciences and engineering to capture phenomena over a broad range of spatial-temporal scales and for accounting for uncertainties [20, 29]. This includes complex fluids and soft materials [9], climatology and weather prediction [15, 48], neuroscience [18], and engineered mechanical and electrical systems [17, 20, 21, 29]. Significant computational expenses in simulations are incurred from the wide range of temporal and spatial scales that must be resolved [4, 5, 48, 53, 60, 62]. Strategies for grappling with these issues include using asymptotic reduced-order modeling approaches for averaging and explicitly removing fast-degrees of freedom [7, 40, 47, 55, 60], coarse-grained modeling to formulate simplified descriptions [30, 44, 66], and analysis to develop numerical methods for handling sources of stiffness [5, 6, 12, 24]. In the stochastic setting this is further complicated by the presence of random perturbations from forcing terms or boundary conditions and the propagation of fluctuations [3, 5, 20, 29, 60].

We develop a class of numerical methods for stiff stochastic systems that preserve statistical structures for time-varying linear operators of the form $d\mathbf{z}_t = L(t)\mathbf{z}_t dt + \mathbf{f}(t)dt + Q(t)d\mathbf{W}_t$. By using Duhamel's principle [25, 34, 58] and Ito calculus [20, 45], we develop ways to analytically integrate stiff parts of the stochastic dynamics. We develop methods for handling cases when the operator L can depend on time and may not commute in the sense $L(t_1)L(t_2) \neq L(t_2)L(t_1)$, which poses challenges for numerical integration. Even in the deterministic setting with $\mathbf{f} = 0$ and $Q(t) = 0$, a non-commuting $L(t)$ raises challenges. In this case, the solution operator $\mathcal{S}$ with $\mathbf{z}(\tau_2) = \mathcal{S}(\tau_1, \tau_2)\mathbf{z}(\tau_1)$ is no longer simply the exponential $\exp\left(\int_{\tau_1}^{\tau_2} L(s)ds\right) \neq \mathcal{S}(\tau_1, \tau_2)$. As an alternative, we represent the solution operator as $\mathcal{S}(\tau_1, \tau_2) = \exp\left(\Omega(\tau_1, \tau_2)\right)$ where we solve a system of dynamical equations to obtain $\Omega(\tau_1, \tau_2) = \sum_{k=1}^{\infty} \Omega_k(\tau_1, \tau_2)$ as a Magnus Expansion [39].

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To develop effective numerical methods for stiff stochastic systems requires handling the stochastic forcing terms and the propagation of fluctuations. In our numerical methods, we approximate the solution map using truncated expansions $\tilde{\Omega}(\tau_1,\tau_2) = \sum_{k=1}^{n} \Omega_k(\tau_1,\tau_2)$ to obtain $\tilde{\mathcal{S}}(\tau_1,\tau_2) = \exp\left(\tilde{\Omega}(\tau_1,\tau_2)\right)$. As a consequence from truncation errors, this augments the temporal evolution and propagation of fluctuations for the discretized stochastic system relative to the continuous dynamics. To mitigate such discretization artifacts in the propagation of fluctuations, we develop stochastic numerical methods that produce marginal statistics having a controlled level of accuracy. We perform stochastic analysis of our exponential integrators to establish explicit relationships between choices for our stochastic driving terms in discretizations and the marginal statistics. For dissipative systems, our methods are related to the balance in statistical mechanics between fluctuations and the dissipation which determines the stationary statistics. We leverage these relationships to develop discretizations for stochastic numerical methods we refer to as *Exponential Fluctuation-Dissipation Discretizations (EFDDs)*.

We show how our EFDD approaches can be used to develop stiff stochastic numerical integrators for systems having stationary and time-varying operators for Stochastic Differential Equations (SDEs) and Stochastic Partial Differential Equations (SPDEs). We present results motivated by SDEs arising in particle simulations and Langevin dynamics. We also give results for SPDEs for fluctuations of concentration fields in spatially-extended systems on deforming domains discretized in time-varying coordinate frames. Our introduced EFDD approaches provide for stochastic dynamical systems general methods for discretization and development of stochastic numerical integration methods for preserving statistical structures while handling stiffness.

Previous early work on exponential integration methods focused on deterministic ODE dynamics $d\mathbf{w}_t/dt = L_0\mathbf{w}_t$, with stationary operators $L(t) = L_0$, [24, 41, 50]. These works have been motivated by the method of integrating factor and rely on the solution map $\mathbf{w}(\tau_2) = \mathcal{S}(\tau_1,\tau_2) = \exp\left((\tau_2-\tau_1)L_0\right)\mathbf{w}(\tau_1)$. A central challenge in such exponential time-stepping methods is to compute efficiently the matrix exponentials [22, 31, 42, 68]. Strategies include projections and preconditioners [35,56,64], using contour integration or expansion identities [37,54], and factorizations [5,19,27,70]. In the case L is low dimensional or can be readily diagonalized, such as with Fast Fourier Transforms [16, 57], the matrix exponential can be computed efficiently. Exponential integrators for determinstic systems using related approaches have been developed in [10, 33, 41, 46, 56]. Work has also been done on developing deterministic exponential integrators for the time-dependent $L(t)$ case [8, 10, 11, 38, 39, 61, 65]. This has in part been motivated by perturbation theory in quantum mechanics [23, 32, 39, 52, 59]. The quantum non-autonomous case served as the early motivation for the Magnus Expansion [39], which we shall utilize for our stochastic methods.

For stochastic systems (SDEs/SPDEs), additional issues arise in handling the contributions of the fluctuations [3–5, 49]. Work on stochastic exponential integrators for stationary operators $L(t) = L_0$ has been done in [1, 5, 21, 28]. In these works, stochastic and conventional integral expressions are derived with terms exponential in the evolution operator. The integrals and exponentials are either analytically computed, such as using diaognalization in an eigenbasis [5], or approximated using Krylov subspaces [21], finite elements [28, 36], or other methods [1, 21]. Exponential integrators have also been developed for non-autonomous stochastic systems permitting non-commuting evolution operators in [2, 13, 26, 36, 67, 69]. In these works, iterated stochastic integrals are derived and approximated with quadratures [26, 69], approximated by solving auxillary equations [67], or other methods [36, 43].

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Our work addresses the issue of preserving statistic structures when performing these exponential discretizations. We also provide for a class of SDEs/SPDEs alternative methods without the need to evaluate directly the stochastic integrals arising in other methods. Our work is motivated by the issue that any approximations introduced for the evolution maps $\mathcal{S}(\tau_1, \tau_2)$ will have implications for how fluctuations propagate in the stochastic system. To ensure good behaviors for the fluctuations, this requires compatibility between the choice of numerical approximation and the way in which the stochastic contributions are approximated. We establish explicit relationships between the choice of approximation for the evolution map and the resulting statistics of the stochastic numerical methods. This can be utilized to develop methods to determine stochastic driving terms in the discretizations that are ensured to produce well-controlled accuracy for important statistics of the system. Our approaches allow for avoiding the iterated stochastic integrals that arise in other methods [26]. In our work, we utilize known information about marginal statistics in the linearized regime to derive the stochastic terms. For both SDEs and SPDEs, our approaches provide principled ways to develop stochastic numerical methods taking discretization artifacts into account in the propagation of fluctuations to ensure preservation of statistical structures while handling stiffness.

Our paper is organized as follows. In section 2, we discuss our general approaches for obtaining stochastic exponential integration methods based on Duhamel's principle and Magnus Expansions. In section 3, we discuss how to determine the stochastic driving terms by performing analysis to establish explicit relationships between the choice of discretizations and resulting marginal statistics. In section 4, we present results for our methods for stiff SDEs and SPDEs making comparisons with non-exponential stochastic numerical methods. In section 4.2, we present results for SDEs including for systems arising in particle simulations and for Langevin dynamics with time-dependent operators. In section 4.3, we show how our approaches can be used to approximate SPDEs which require choices for both the spatial and temporal discretizations. We show how methods can be developed for SPDEs modeling fluctuations of concentration fields in spatially-extended systems on deforming domains discretized in time-varying coordinate frames. For time-varying stochastic dynamical systems, our introduced discretization approaches provide for SDEs and SPDEs general exponential numerical integrators for preserving statistical structures while handling stiffness.

2 Stochastic Exponential Integrators for Stationary and Time-Varying Dissipative Operators $L(t)$

We develop exponential intergators for time-varying stochastic dynamical systems of the form

$$d\mathbf{z}_t = L(t)\mathbf{z}_t dt + \mathbf{f}(t)dt + Q(t)d\mathbf{W}_t. \tag{1}$$

By Duhamel's Principle [25, 58] the solution can be expressed as

$$\mathbf{z}(\tau_2) = \mathcal{S}(\tau_2, \tau_1)\mathbf{z}(\tau_1) + \int_{\tau_1}^{\tau_2} \mathcal{S}(\tau_2, s)\mathbf{f}(s)ds + \mathbf{\Xi}_{\tau_1,\tau_2}. \tag{2}$$

The $\mathcal{S}(\tau_2, \tau_1)$ is the solution map of $d\mathbf{w}_t = L(t)\mathbf{w}_t dt$, when starting with initial condition $\mathbf{w}(\tau_1)$ yielding $\mathbf{w}(\tau_2) = \mathcal{S}(\tau_2, \tau_1)\mathbf{w}(\tau_1)$. The $\mathbf{\Xi}_{\tau_1,\tau_2}$ is a Gaussian random variable given by

$$\mathbf{\Xi}_{\tau_1,\tau_2} = \int_{\tau_1}^{\tau_2} \mathcal{S}(\tau_2, s)Q(s)d\mathbf{W}_s. \tag{3}$$

In the case when $\mathbf{f} = 0$, it can be shown the mean of $\mathbf{\Xi}_{\tau_1,\tau_2}$ is zero, and the covariance can be expressed as

$$\langle \mathbf{\Xi}_{\tau_1,\tau_2} \mathbf{\Xi}_{\tau_1,\tau_2}^T \rangle = C(\tau_2) - \mathcal{S}(\tau_2,\tau_1) C(\tau_1) \mathcal{S}(\tau_2,\tau_1)^T, \tag{4}$$

where $C(s) = \langle \mathbf{z}(s)\mathbf{z}(s)^T \rangle$. This uses that $\mathbf{z}(s)$ is Markovian and $\langle (\mathbf{z}(\tau_1)\mathbf{\Xi}_{\tau_1,\tau_2} \rangle = 0$. For physical systems arising in statistical mechanics, all dissipative contributions to the dynamics are assumed to be modeled by $\mathcal{L}(t)$ with $\mathbf{f}(t)$ acting as an external forcing. In this case, even when $\mathbf{f} \neq 0$, the $\mathbf{\Xi}_{\tau_1,\tau_2}$ is given by the fluctuations in equation 4.

In the stationary case with $L(t) = L_0$, this simplifies with $\mathcal{S}(\tau_2,\tau_1) = \exp\left(\int_{\tau_1}^{\tau_2} L_0 \, ds\right) = \exp\left((\tau_2 - \tau_1)L_0\right)$. In the case that $L(t_1)L(t_2) = L(t_2)L(t_1)$, $\forall t_1, t_2$, the solution map also simplifies and can be expressed as $\mathcal{S}(\tau_2,\tau_1) = \exp\left(\int_{\tau_1}^{\tau_2} L(s) \, ds\right)$. However, in the general case when the operators do not commute, $\exists t_1, t_2$ with $L(t_1)L(t_2) \neq L(t_2)L(t_1)$, the integral expression is no longer valid, and we can have $\mathcal{S}(\tau_2,\tau_1) \neq \exp\left(\int_{\tau_1}^{\tau_2} L(s) \, ds\right)$. Fortunately, there are still alternative ways to exponentiate $L(t)$ to express the solution map as $\mathcal{S}(\tau_2,\tau_1) = \exp\left(\Omega(\tau_2,\tau_1)\right)$, where $\Omega = \sum_{k=1}^{\infty} \Omega_k$ is a Magnus Expansion for $L(t)$ [39]. This will provide the basis for our development of exponential integration methods and discretizations for time-varying stochastic systems.

2.1 Magnus Expansions

To motivate the expansions, we first consider the homogeneous system

$$d\mathbf{w}_t = L(t)\mathbf{w}_t dt, \tag{5}$$

with the deterministic and stochastic driving terms absent. Let the commutator be denoted by $[L(t_1), L(t_2)] = L(t_1)L(t_2) - L(t_2)L(t_1)$. We consider the case when for some t_1, t_2 we have $[L(t_1), L(t_2)] \neq 0$. The solution to equation 5 in principle can be expressed as the time-ordered exponential

$$\mathbf{w}(t) = \mathcal{T}\left\{\exp\left(\int_0^t L(s)ds\right)\right\}\mathbf{w}_0. \tag{6}$$

The time-ordered exponential is by definition

$$\mathcal{T}\left\{\exp\left(\int_0^t L(s)ds\right)\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^t \cdots \int_0^t \mathcal{T}\left[L(t_1), L(t_2), \ldots, L(t_n)\right] \, dt_1 \cdots dt_n \tag{7}$$

$$= \sum_{n=0}^{\infty} \int_0^t \int_0^{t_n'} \cdots \int_0^{t_2'} L(t_n'), L(t_{n-1}'), \ldots, L(t_1') \, dt_1' \cdots dt_n'. \tag{8}$$

The ordering operation $\mathcal{T}$ arranges the terms in the product so that from right to left they involve the terms increasing in time. For example, with $t_1 < t_2 < t_3$, the $\mathcal{T}[L(t_1)L(t_3)L(t_2)] = L(t_3)L(t_2)L(t_1)$. While truncations of this expansion can be computed in principle, this can be inefficient and cumbersome, especially when L commutes for a significant range of times t.

As an alternative, we use an expansion given in terms of the commutators of $L(t_k)$, referred to as a Magnus Expansion [39]. Using this approach, the solution to equation 5 can be written as the

standard exponential (unordered) with the infinite series

$$\mathbf{w}(t) = \exp\left(\Omega(t,0)\right)\mathbf{w}_0, \quad \Omega(t,0) = \sum_{k=1}^{\infty} \Omega_k(t,0). \tag{9}$$

In the expansion the terms are given by integrals of L and its commutators as

$$\Omega_1(t_2,t_1) = \int_{t_1}^{t_2} ds_1 L(s_1), \quad \Omega_2(t_2,t_1) = \frac{1}{2!}\int_{t_1}^{t_2} ds_1 \int_{t_1}^{s_1} ds_2 [L(s_1), L(s_2)], \tag{10}$$

$$\Omega_3(t_2,t_1) = \frac{1}{3!}\int_{t_1}^{t_2} ds_1 \int_{t_1}^{s_1} ds_2 \int_{t_1}^{s_2} ds_3 \Big(\big[L(s_1), [L(s_2), L(s_3)]\big] + \big[L(s_3), [L(s_2), L(s_1)]\big] \Big). \tag{11}$$

This can be expressed more concisely using recursion and defining the iterated commutator (adjoint endomorphism) ad_Ω^k with $\mathrm{ad}_\Omega^0(L) = L$ and $\mathrm{ad}_\Omega^k(L) = [\Omega, \mathrm{ad}_\Omega^{k-1}(L)]$. As notational convention, we will use $\mathrm{ad}_\Omega(L) = \mathrm{ad}_\Omega^1(L) = [\Omega, L]$. The terms of the Magnus Expansion can be expressed as

$$\Omega_k(t_2,t_1) = \sum_{\ell=1}^{k-1} \frac{B_\ell}{\ell!} \sum_{i_1+\cdots i_\ell = k-1, i_1 \geq 1, \ldots, i_\ell \geq 1} \int_{t_1}^{t_2} \mathrm{ad}_{\Omega_{i_1}(t_1,s)}(L) \cdots \mathrm{ad}_{\Omega_{i_\ell}(t_1,s)}(L)\; L(s)\; ds,$$

where $k \geq 2$ and B_ℓ is the ℓ^{th} Bernoulli number [14] defined by $x/(e^x - 1) = \sum_{\ell=0}^{\infty} B_\ell \frac{x^\ell}{\ell!}$.

From our derivations for SDEs based on Duhamel's Principle [25, 58], we can approximate for a finite time-step the stochastic dynamics as

$$\mathbf{z}_{n+1} = \exp\left(\tilde{\Omega}(t_{n+1}, t_n)\right)\mathbf{z}_n + \int_{t_n}^{t_{n+1}} \exp\left(\tilde{\Omega}(t_{n+1}, s)\right)\mathbf{f}(s) ds + \boldsymbol{\Xi}_n, \tag{12}$$

where $\tilde{\Omega}(t,s) = \sum_{k=1}^{n_b} \Omega_k(t,s)$ is the truncated Magnus expansion at order n_b. The $\boldsymbol{\Xi}_n$ is a Gaussian random variable with mean $\mathbf{0}$. In the case with $\mathbf{f} = 0$, the covariance can be expressed as

$$\langle \boldsymbol{\Xi}_n \boldsymbol{\Xi}_n{}^T \rangle = C_{n+1} - \exp\left(\tilde{\Omega}(t_{n+1}, t_n)\right) C_n \exp\left(\tilde{\Omega}(t_{n+1}, t_n)\right)^T, \tag{13}$$

where $C_n = \langle \mathbf{z}_n \mathbf{z}_n^T \rangle$. We derived this using Ito's Isometry [45]. From the dynamics over time t_n to t_{n+1}, we have $C_{n+1} = \langle \mathbf{z}_{n+1} \mathbf{z}_{n+1}^T \rangle = \exp\left(\tilde{\Omega}(t_{n+1}, t_n)\right) C_n \exp\left(\tilde{\Omega}(t_{n+1}, t_n)\right)^T + \langle \boldsymbol{\Xi}_n \boldsymbol{\Xi}_n{}^T \rangle$. Given this relationship between C_{n+1} and C_n, this ensures the RHS is always positive semi-definite for any covariance C_n.

For some stochastic systems, it may be natural to try to ensure for the discretization a prescribed target marginal distribution is obtained that is Gaussian with covariance $\tilde{C}_n$, so that $\langle \mathbf{z}_n \mathbf{z}_n^T \rangle = \tilde{C}_n$ for each n. In this case it is natural to ask what conditions are required on the sequence $\{C_n\}_{n=1}^{\infty}$ to ensure there exists a $Q(t)$ achieving this outcome. The forcing term is always a Gaussian and can be expressed as $\boldsymbol{\Xi}_n = Q_n \xi_n$ where $\xi_n \sim \eta(0,1)$ with the standard Gaussian denoted by $\eta(0,1)$. This requires

$\langle \boldsymbol{\Xi}_n \boldsymbol{\Xi}_n{}^T \rangle = Q_n Q_n^T = C_{n+1} - \exp\left(\tilde{\Omega}(t_{n+1}, t_n)\right) C_n \exp\left(\tilde{\Omega}(t_{n+1}, t_n)\right)^T$ and that this be symmetric and positive semi-definite.

In the special case when $\tilde{\Omega}$ and C diagonalize in the same basis, this condition can be expressed as

$$\log\left(\frac{\lambda_i(C_{n+1})}{\lambda_i(C_n)}\right) \geq 2\lambda_i\left(\tilde{\Omega}(t_{n+1},t_n)\right), \quad \forall i. \tag{14}$$

The eigenvalues are taken to be indexed in i by ordering from largest to smallest using $\lambda(C_{n+1})$. Since C_n are covariances, we have $\lambda_i(C_k) \geq 0$. When $\tilde{\Omega}$ is strictly dissipative, we have $\lambda_i(\tilde{\Omega}) < 0$. We see a sufficient criteria for the condition 14 to hold is that the sequence of eigenvalues $\{C_n\}_{n=1}^{\infty}$ be increasing or constant (non-decreasing). More generally, the condition 14 requires the covariance not decrease too rapidly, for instance when approaching a stationary state $C_n \to C_\infty$. These results provide guidelines when developing effective stochastic numerical discretizations for preserving the statistical structures represented by $\{C_n\}_{n=1}^{\infty}$. In statistical mechanics, for the linearized system the marginals of the stationary distributions are often known. We develop approaches for using this in the design of discretizations and integrators.

3 Integrators Satisfying Fluctuation-Dissipation Balance

In linear stochastic systems the dissipation and fluctuations of the system balance to yield the stationary distribution. For a stationary disspative operator $L(t) = L_0$, $Q(t) = Q_0$ and dynamics

$$d\mathbf{z}_t = L\mathbf{z}_t dt + Qd\mathbf{W}_t \tag{15}$$

, the covariance $C(t) = \langle \mathbf{z}_t \mathbf{z}_t^T \rangle \to C_\infty = C$ as $t \to \infty$. We have from Ito Calculus [45] the relationship

$$QQ^T = -LC - CL^T. \tag{16}$$

For the stationary covariance C, this gives the relationship to the fluctuations Q and dissipation L of the system. In statistical mechanics this is referred to as fluctuation-dissipation balance [51].

We can establish similar relations to take into account temporal discretizations of the dynamics to ensure fluctuation-dissipation balance in our numerical methods. Consider the Euler-Marayuma discretization

$$\mathbf{z}_{n+1} = \mathbf{z}_n + L\mathbf{z}_n\Delta t + Q\Delta W_n, \tag{17}$$

where $\Delta W_n = \sqrt{\Delta t}\xi$ with $\xi \sim \eta(0,1)$. In this case, we take Q so that

$$QQ^T = -LC - CL^T - \Delta t LCL^T. \tag{18}$$

This choice of Q ensures even with the temporal discretization errors governed by the time-scale Δt, the stationary fluctuations of the system will still have covariance C.

In the case of exponential integration with stationary dissipative operators $L(t) = L_0$ and covariance C, we generalize this. Let $\tilde{\exp}(\Delta t L)$ denote a numerical approximation of the matrix exponential $\exp(\Delta t L)$. For $\mathbf{z}_{n+1} = \mathbf{z}(t_{n+1})$ we discretize in time using

$$\mathbf{z}_{n+1} = \tilde{\exp}(\Delta t L)\mathbf{z}_n + \int_{t_n}^{t_{n+1}} \tilde{\exp}((t_{n+1}-s)L)\mathbf{f}(s)ds + \mathbf{\Xi}_n, \tag{19}$$

where $\boldsymbol{\Xi}_n$ is a Gaussian with mean 0 and covariance

$$\langle \boldsymbol{\Xi}_n {\boldsymbol{\Xi}_n}^T \rangle = C - \tilde{\exp}(\Delta t L) C \tilde{\exp}(\Delta t L)^T. \tag{20}$$

This choice for $\boldsymbol{\Xi}_n$ ensures when $\mathbf{f} = 0$ the stationary fluctuations of the system will still have covariance C despite the numerical discretization errors introduced by the approximate exponentials $\tilde{\exp}(\Delta t L)$. For our numerical methods to be able to achieve the fluctuation-dissipation balance property, an important requirement is the numerical approximations $\tilde{\exp}$ yield covariance expressions in equation 20 that are positive semi-definite.

In the case of exponential intergation with $L(t)$ that commutes in time, $L(t_1)L(t_2) = L(t_2)L(t_1)$, $\forall t_1, t_2$, we let $A(t,s) = \int_s^t L(r)dr$. In practice, this will be approximated by quadratures to yield $\tilde{A}(t,s)$. We discretize the system in time using

$$\mathbf{z}_{n+1} = \exp\left(\tilde{A}(t_{n+1}, t_n)\right)\mathbf{z}_n + \int_{t_n}^{t_{n+1}} \exp\left(\tilde{A}(t_{n+1}, s)\right)\mathbf{f}(s)ds + \boldsymbol{\Xi}_n, \tag{21}$$

where $\boldsymbol{\Xi}_n$ is a Gaussian with mean 0 and covariance

$$\langle \boldsymbol{\Xi}_n {\boldsymbol{\Xi}_n}^T \rangle = C - \exp\left(\tilde{A}(t_{n+1}, t_n)\right) C \exp\left(\tilde{A}(t_{n+1}, t_n)\right)^T. \tag{22}$$

This choice for $\boldsymbol{\Xi}_n$ again ensures despite numerical discretization errors that when $\mathbf{f} = 0$ the stationary fluctuations of the system will have covariance C.

In the case of exponential integration with an $L(t)$ that does not commute, $L(t_1)L(t_2) \neq L(t_2)L(t_1)$, we discretize the system in time using

$$\mathbf{z}_{n+1} = \tilde{\exp}(\tilde{\Omega}(t_{n+1}, t_n))\mathbf{z}_n + \int_{t_n}^{t_{n+1}} \tilde{\exp}(\tilde{\Omega}(t_{n+1}, s))\mathbf{f}(s)ds + \boldsymbol{\Xi}_n, \tag{23}$$

where $\tilde{\Omega}(t,s) = \sum_{k=1}^{n_b} \Omega_k(t,s)$ is the truncated Magnus expansion at order n_b and $\tilde{\exp}$ are approximate exponentials. The $\boldsymbol{\Xi}_n$ is a Gaussian random variable with mean 0 with covariance

$$\langle \boldsymbol{\Xi}_n {\boldsymbol{\Xi}_n}^T \rangle = C - \tilde{\exp}\left(\tilde{\Omega}(t_{n+1}, t_n)\right) C \tilde{\exp}\left(\tilde{\Omega}(t_{n+1}, t_n)\right)^T. \tag{24}$$

This choice for $\boldsymbol{\Xi}_n$ ensures even when $L = L(t)$ and there are numerical discretization artifacts from $\tilde{\exp}$ and from truncating the expansion to $\tilde{\Omega}$, when $\mathbf{f} = 0$ the stationary fluctuations of the system will still have covariance C. These methods provide ways to handle the stochastic dynamics of SDEs of the form in equation 1 with exponential integration while satifying the fluctuation-dissipation balance property up to round-off errors.

Our fluctuation-dissipation balance approaches can also be used for taking into account for SPDEs the spatial numerical discretization errors to ensure good behaviors for the propagation of fluctuations. Consider SPDEs of the general form

$$dw_t = \mathcal{L}(t)w_t dt + f_t dt + d\mathcal{Q}(t)d\mathcal{W}_t, \tag{25}$$

where $\mathcal{W}_t = \mathcal{W}(t, \mathbf{x}; \omega)$ is a Wiener stochastic field with sample point ω, and $w_t = w(\mathbf{x}, t; \omega)$, $f_t = f(\mathbf{x}, t; \omega)$ are stochastic fields. The $\mathcal{L}$ and $\mathcal{Q}$ are linear operators, which can include operations such as differentiation. In this case, a semi-discretization first would be performed spatially to

obtain a finite dimensional representation of the fields $w_t \approx \mathbf{z}_t$, $f_t \approx \mathbf{f}(t)$ and the operators with $\mathcal{L}(t) \approx L(t)$ and $\mathcal{Q}(t) \approx Q(t)$. This reduces SPDEs of the form of equation 25 to SDEs of the form in equation 1. We can then apply our discretization approaches to obtain numerical methods achieving fluctuation-dissipation balance. We refer to this class of methods as Exponential Fluctuation Dissipation Discretizations (EFDDs). Our methods provide ways to discretize time-varying stochastic systems with exponential integration while preserving statistical structures associated with fluctuation-dissipation balance.

4 Results

We now show in practice how our exponential integration methods and fluctuation-dissipation discretization approaches can be used in practice on a few example stochastic systems.

4.1 Oscillating Stochastic System with Time-Varying $L(t)$

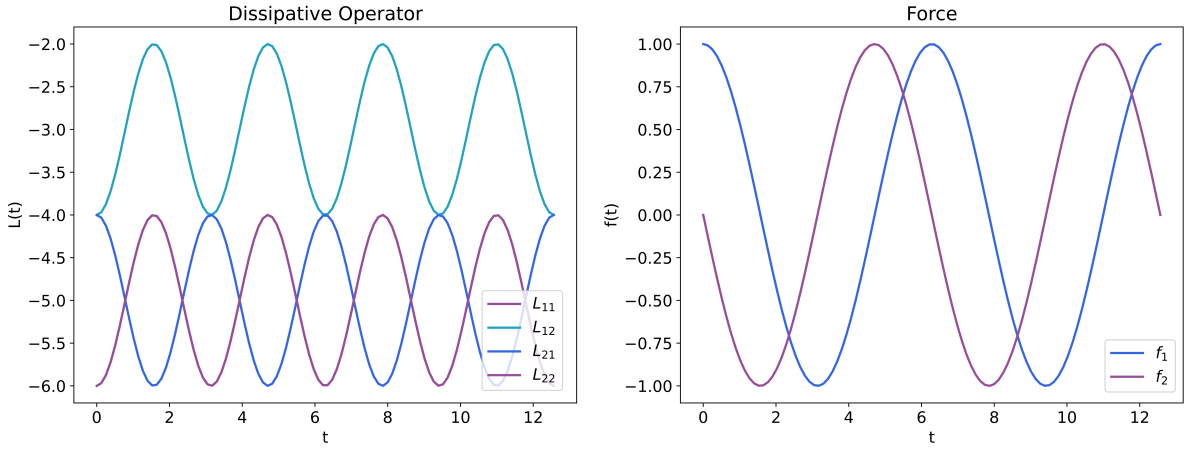

Figure 1: ***Operator and Force Components.*** *The components of the dissipative operator $L(t)$ (left) and the time-dependent force $\mathbf{f}(t)$ (right). The parameters are $\gamma = 2$, $\omega = 1$.*

We demonstrate our exponential integration approach and its performance for a stochastic system with time-varying operators of the form $d\mathbf{z}_t = L(t)\mathbf{z}_t dt + \mathbf{f}(t)dt + Q(t)d\mathbf{W}_t$, where

$$L(t) = -\gamma \begin{bmatrix} 2+\cos^2(\omega t) & 2-\sin^2(\omega t) \\ 2+\sin^2(\omega t) & 2+\cos^2(\omega t) \end{bmatrix}, \ \mathbf{f}(t) = \omega \begin{bmatrix} \cos(\omega t) \\ -\sin(\omega t) \end{bmatrix}, \ C = \begin{bmatrix} c_1 & 0 \\ 0 & c_2 \end{bmatrix}. \tag{26}$$

For the SDE we take $Q(t) = -L(t)C - CL(t)^T$. We compare the accuracy of our exponential integration methods with the Euler-Maruyama Method as the time-step Δt is varied, see Figure 2.

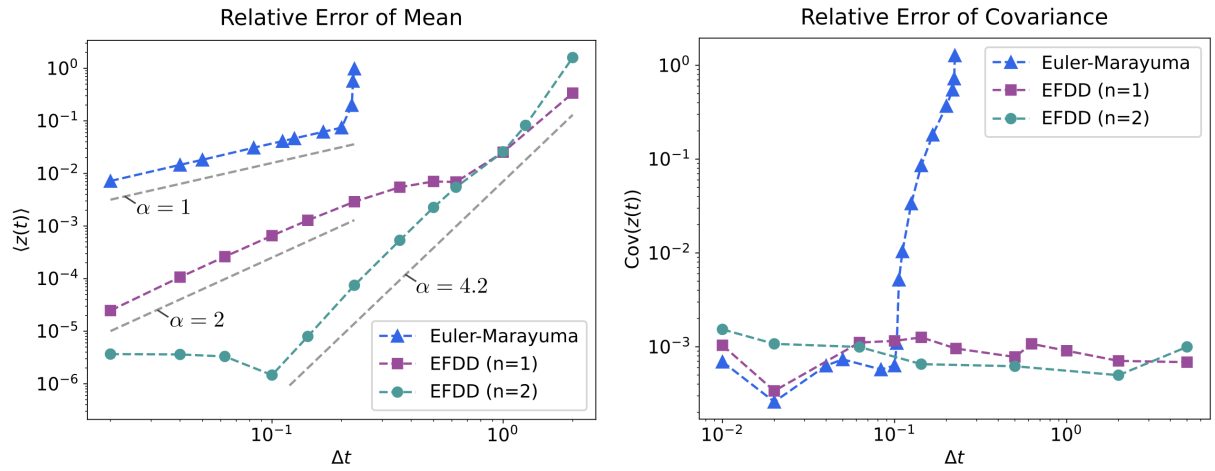

Figure 2: ***Accuracy of Methods.*** *We compare our stochastic magnus exponential integrator methods with Euler-Marayuma methods [29] for the SDE in equation 33. We compare the relative errors of* $\mathbf{z}(t)$ *for the mean (left) and the covariance (right). We find our methods with* $n = 2$ *exhibit fourth-order accuracy errors* $O(\Delta t^{\alpha})$ *with* $\alpha \sim 4.2$ *and for* $n = 1$ *second-order accuracy* $\alpha \sim 2$*. This is in contrast the Euler-Marayuma method that exhibits here only first-order accuracy* $\alpha \sim 1$*. Our methods also exhibit stability and accuracy over a wider range of time-steps* Δt*. We find here our exponential integrator gives an accuracy slightly better than fourth-order* $\alpha = 4.2$ *given the additional non-linear contributions of the exponentials relative to Taylor expansions. Parameters for the SDE in equation 26 were* $\gamma = 2$*,* $\omega = 1$*,* $c_1 = 0.04$*,* $c_2 = 0.05$*,* $t_f = 5$*, and* $\mathbf{z}_0 = [1, 1]^T$*.*

Since the stochastic process $\mathbf{z}(t)$ has a Gaussian distribution at each time, we can assess the accuracy of the numerical methods in approximating the marginal distribution mean and covariance at the final time t_f using $\mathbf{z}(t_f)$. From Figure 2, we see that our exponential integration methods are able to integrate accurately over an order-of-magnitude larger Δt compared to the Euler-Maruyama Method. Explicit Euler methods are well-known to have stability constraints $\Delta t \leq \tau = 2/|\lambda|$, where λ is the largest eigenvalue of L. From an analysis of $L(t)$ we have $\tau = 0.2$, which matches where we see the Euler-Marayuma Method become unstable. We also see for Euler-Marayuma as Δt approaches τ the covariance also degrades in accuracy, which manifests as a break-down of the positive semi-definiteness of the covariance in equation 24, see Figure 2.

We further find that our exponential integration methods (EFDDs) exhibit second-order rate of convergence. This is in contrast to the Euler-Maruyama Method which exhibits only first-order accuracy, see Figure 2. Our exponential integration methods (EFDDs) are able to maintain both stability and accuracy for time-steps Δt about two to three orders of magnitude beyond the Euler-Maruyama Method.

4.2 Langevin Dynamics in a Moving Reference Frame

We consider simulations of a particle system with inertial Langevin Dynamics in a moving reference frame. For fixed stationary coordinates, the dynamics can be expressed as $d\mathbf{z}_t = L\mathbf{z}_t dt + Q d\mathbf{W}_t$,

where $\mathbf{z}_t = (x, v_x, y, v_y)^T$, and

$$L = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -K/m & -\gamma/m & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -K/m & -\gamma/m \end{bmatrix}, \; Q = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \sqrt{2k_BT\gamma}/m & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2k_BT\gamma}/m \end{bmatrix}. \tag{27}$$

The (x, y) gives the particle location and (v_x, v_y) the particle velocity. This gives dynamics for particles of mass m diffusing in the harmonic potential $U(\mathbf{x}) = \frac{1}{2}K\mathbf{x}^2$, which corresponds to the Ornstein-Uhlenbeck process [63]. The k_BT gives the thermal energy with k_B Boltzmann's constant and T the temperature. The "$Qd\mathbf{W}_t/dt$" gives the stochastic force associated with thermal fluctuations and K the harmonic spring stiffness. At equilibrium the particle degrees of freedom fluctuate with the Gibbs-Boltzmann distribution with mean zero and covariance

$$C = \begin{bmatrix} k_BT/K & 0 & 0 & 0 \\ 0 & k_BT/m & 0 & 0 \\ 0 & 0 & k_BT/K & 0 \\ 0 & 0 & 0 & k_BT/m \end{bmatrix}. \tag{28}$$

Suppose we consider the same dynamics, but modeled in a rotating coordinate frame given by the following time-dependent transformation

$$\begin{bmatrix} \tilde{x} \\ \tilde{y} \end{bmatrix} = \begin{bmatrix} \cos(\theta(t)) & \sin(\theta(t)) \\ -\sin(\theta(t)) & \cos(\theta(t)) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}. \tag{29}$$

The $\theta(t)$ gives the time-dependent angle of the rotation. From Ito's Lemma, the stochastic dynamics in the coordinates $\tilde{\mathbf{z}} = (\tilde{x}, \tilde{v}_x, \tilde{y}, \tilde{v}_y)^T$ are given by $d\tilde{\mathbf{z}}_t = \tilde{L}(t)\tilde{\mathbf{z}}_t dt + \tilde{Q}(t)d\mathbf{W}_t$. This can be expressed as $\tilde{\mathbf{z}}_t = R(t)\mathbf{z}_t$, $\tilde{C}(t) = R(t)CR(t)^T$, $\tilde{L}(t) = \left(\frac{dR}{dt} + R(t)L\right)R(t)^{-1}$, where

$$R(t) = \begin{bmatrix} \cos(\theta(t)) & 0 & \sin(\theta(t)) & 0 \\ -\sin(\theta(t))\dot{\theta}(t) & \cos(\theta(t)) & \cos(\theta(t))\dot{\theta}(t) & \sin(\theta(t)) \\ -\sin(\theta(t)) & 0 & \cos(\theta(t)) & 0 \\ -\cos(\theta(t))\dot{\theta}(t) & -\sin(\theta(t)) & -\sin(\theta(t))\dot{\theta}(t) & \cos(\theta(t)) \end{bmatrix}. \tag{30}$$

We show some sample trajectories of these dynamics in Figure 3.

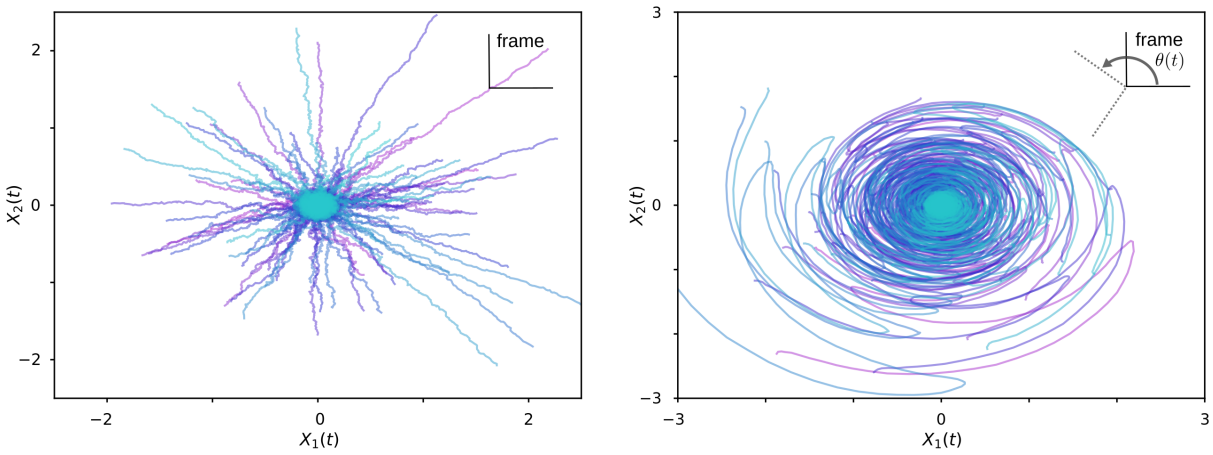

Figure 3: ***Stochastic Dynamics in the Stationary and Rotating Frames.*** *We show how the stochastic dynamics manifests in (left) a stationary reference frame $\theta(t) = 0$, and (right) an oscillating rotating reference frame $\theta(t) = 2 + \cos(\omega t)$, $\omega = 1$.*

We compare our stochastic exponential integrator EFDD with Euler-Maruyama. We simulate stochastic trajectories using time steps Δt over the time $[0, t_f]$. We compute the relative errors in the mean and covariance of $\tilde{\mathbf{z}}(t_f)$. We show how varying Δt impacts the accuracy of the numerical methods in Figure 4. The studies use the following parameter values $K = 2$, $m = 1$, $\omega = 1$, $\gamma = 2.5$, $k_B T = 0.01$, $\theta(t) = 2 + \cos(\omega t)$, $t_f = 4.0$, and $\tilde{\mathbf{z}}_0 = R(0)\left[1, \quad -0.1, \quad 1, \quad -0.1\right]^T$.

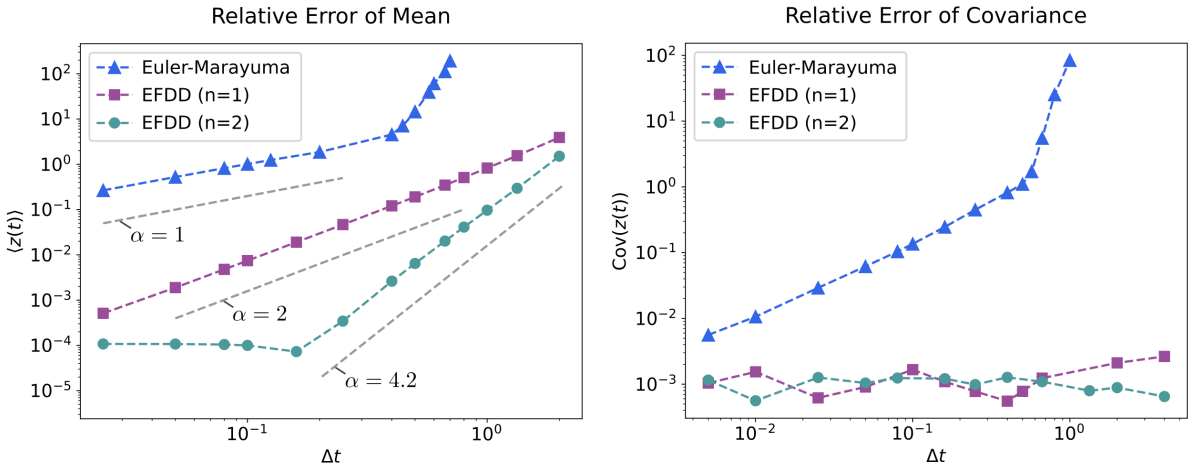

Figure 4: *Accuracy of the mean (left) and covariance (right) of each numerical method. We find our methods with $n = 2$ exhibit fourth-order accuracy errors $O(\Delta t^\alpha)$ with $\alpha \sim 4.2$ and for $n = 1$ second-order accuracy $\alpha \sim 2$. This is in contrast the Euler-Marayuma method that exhibits here only first-order accuracy $\alpha \sim 1$. Our methods also exhibit stability and accuracy over a wider range of time-steps Δt. Results for parameter values $K = 2$, $m = 1$, $\omega = 1$, $\gamma = 2.5$, $k_B T = 0.01$, $\theta(t) = 2 + \cos(\omega t)$, $t_f = 4$, and $\tilde{\mathbf{z}}_0 = R(0)[1.0, -0.1, 1.0, -0.1]^T$.*

We find our EFDDs exhibit second-order convergence relative to Euler-Marayuma. We

also find our EFDD methods are also stable over a wider range of Δt. Since the $\tilde{L}(t)$ is diagonalizable for all t values, the critical time-scale for stability of the Euler-Maruyama method is $\tau = \min_{t\in[0,t_f],\lambda\in\text{eig}(\tilde{L}(t))} \left[-2\text{Re}(\lambda)/\left(\text{Re}(\lambda)^2 + \text{Im}(\lambda)^2\right)\right]$. The λ denotes the eigenvalues of $\tilde{L}(t)$. and the minimum is computed over all t. For the chosen parameters, $\tau \approx 0.53$ giving stability condition $\Delta t \leq \tau$. We find this is close to where we see the empirical accuracy of the Euler-Maruyama degrade with a steeper slope, see Figure 4.

4.3 Stochastic Partial Differential Equation (SPDEs) on Deforming Domains

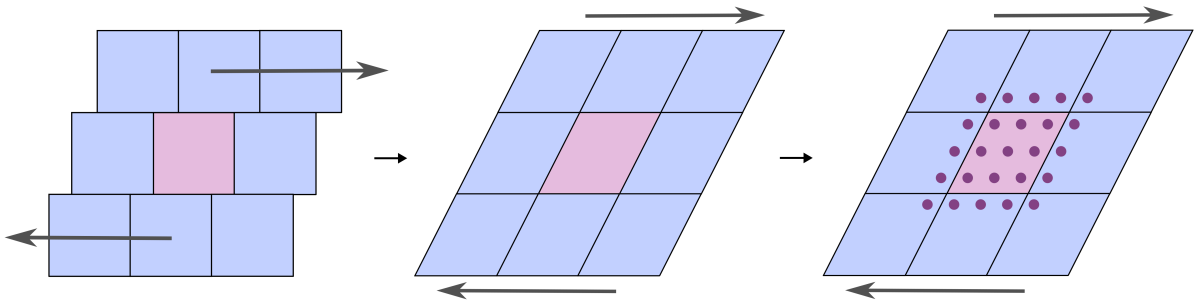

Figure 5: *The boundary conditions can be viewed as modeling a sheared material by shifting the periodic images from the unit cell, giving Lees-Edwards boundary conditions [4] (left). An equivalent way to model the same system is to deform the unit cell and periodic images (middle). The deforming reference frame allows for a discretization avoiding jump conditions but occuring on a moving deforming grid (right).*

In some applications it is natural to approximate SPDEs by discretizations that change over time, see Figure 5 and [4]. For sheared materials, we consider the following class of SPDEs with jump boundary conditions

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = D\Delta u(\mathbf{x},t) + f(\mathbf{x},t) + g_{\text{stoch}}(\mathbf{x},t) \tag{31}$$

$$u(x + X(t), y + L, t) = u(x, y, t) + \mathcal{W}(t). \tag{32}$$

For material points on the boundary, the $X(t) = \int_0^t v(s)ds$ gives the boundary displacement and $v(s)$ the velocity of the shear at the boundary. The $\mathcal{W}(t)$ gives the jump in the field induced by the change in velocity when crossing the boundary, such as the jump that occurs in the velocity field $\mathcal{W}(t) = v(t)$, see Figure 5. For scalar fields typically we will have $\mathcal{W}(t) = 0$.

For a steady deformation, we have $v(s) = \dot{\gamma}L$ at time s for a shear rate of $\dot{\gamma}$ and domain size in each direction L. In oscillatory shear $v(s) = \dot{\gamma}L\sin(\omega s)$ for frequency ω [4]. These SPDEs can be used to describe transport and fluctuations in density, concentrations, or temperature fields in materials with shear modeled by Lees-Edwards boundary conditions [4]. To avoid explicit jumps, we can reformulate the system using a deformed coordinate system and time-dependent grid to accommodate the shift that occurs for the periodic images at the boundary, see Figure 5 and [4].

This yields the reformulated SPDEs for the deforming coordinate frame

$$\frac{\partial w(\tilde{\mathbf{x}},t)}{\partial t} = D\tilde{\Delta}w(\tilde{\mathbf{x}},t) - \frac{x_2}{L}\frac{dX}{dt}\frac{\partial w}{\partial \tilde{x}_1} + g_{\text{stoch}}(\tilde{\mathbf{x}},t) \tag{33}$$

$$w(\tilde{x}_1,\tilde{x}_2+L,t) = w(\tilde{x}_1,\tilde{x}_2,t) + \mathcal{W}(t). \tag{34}$$

The deforming coordinates are given by $\tilde{\mathbf{x}} = \mathbf{x} + (X(t)x_2/L)\mathbf{e}_1$, where shear occurs in the x_1-direction denoted by $\mathbf{e}_1$. The $w(\tilde{x}_1,\tilde{x}_2,t) = u(\tilde{x}_1 + (X(t)x_2/L),\tilde{x}_2,t)$ introducing the source term $-(x_2/L)\frac{dX}{dt}\frac{\partial w}{\partial \tilde{x}_1}$. When $\mathcal{W}(t) = 0$, the boundary conditions for $w(\tilde{\mathbf{x}},t)$ become standard periodic boundary conditions

$$w(x_1,x_2+L,t) = w(x_1,x_2,t). \tag{35}$$

The Laplacian Δ can be expressed in the deforming coordinates as

$$\tilde{\Delta}w(\tilde{\mathbf{x}}) = \left(\delta_{k\ell} + \frac{\delta_{k2}}{L}X(t)\delta_{\ell 1}\right)\frac{\partial}{\partial \tilde{x}_\ell}\left(\left(\delta_{kj} + \frac{\delta_{k2}}{L}X(t)\delta_{j1}\right)\frac{\partial w(\tilde{\mathbf{x}})}{\partial \tilde{x}_j}\right) \tag{36}$$

For the undeformed grid spacing we take $\Delta x = L/N$ and use indexing conventions $\mathbf{m} = (m_1, m_2)$ with $m_i \in [0, 1, \ldots, N-1]$.

This type of discretization results in time-varying stochastic systems of the form

$$d\mathbf{z}_t = L(t)\mathbf{z}_t dt + \mathbf{f}(t)dt + Q(t)d\mathbf{W}_t. \tag{37}$$

This is to be interpreted in the sense of Ito Calculus [45]. The $[\mathbf{z}_t]_{\mathbf{i}} \approx w(\tilde{\mathbf{x}}_{\mathbf{i}},t)$ approximates the field at the discretized locations $\tilde{\mathbf{x}}_{\mathbf{i}}(t)$ of the deforming grid. The $L(t)$ denotes a dissipative operator having negative eigenvalues, $\mathbf{f}(t)$ is a time-dependent forcing term, $Q(t)$ is a linear operator determining the stochastic driving field approximating $Qd\mathbf{W}_t \approx g_{\text{stoch}}$, with $d\mathbf{W}_t$ increments of Brownian motion.

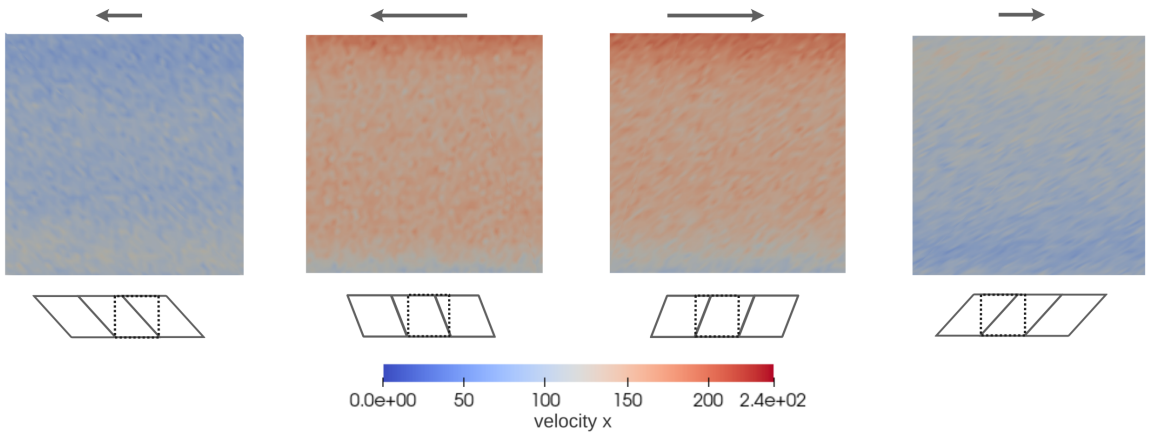

Figure 6: ***Concentration Field Fluctuations on a Shearing Domain.*** *The SPDE is solved on a shear deforming domain resulting in discreteizations with operators $L(t)$ and $Q(t)$. Shown is the x-component of the velocity for a given deformation of the field on the unit cell (dotted lined box). We use the periodicity of the solution on the deformed domain (solid line boxes).*

We descretize the operators using finite difference methods. For computing exponentials of operators we use the discrete Fourier transforms

$$\hat{w}_{\mathbf{k}} = \frac{1}{N^2} \sum_{\mathbf{m}} w_{\mathbf{m}} \exp\left(-i2\pi \mathbf{k} \cdot \mathbf{m}/N\right), \qquad w_{\mathbf{m}} = \sum_{\mathbf{k}} \hat{w}_{\mathbf{k}} \exp\left(i2\pi \mathbf{k} \cdot \mathbf{m}/N\right). \tag{38}$$

The target equilibrium covariance will be represented as

$$C_{\mathbf{k}\mathbf{k}'}(t) = \left\langle \left(\hat{w}_{\mathbf{k}} - \langle \hat{w}_{\mathbf{k}} \rangle\right) \overline{\left(\hat{w}_{\mathbf{k}'} - \langle \hat{w}_{\mathbf{k}'} \rangle\right)} \right\rangle. \tag{39}$$

To ensure that $w_{\mathbf{m}}$ is real-valued, the complex-valued Gaussian increments $dW_{\mathbf{k}}$ must satisfy $dW_{\mathbf{k}} = \overline{dW_{\mathbf{N}-\mathbf{k}}}$. To generate complex-valued standard normal Gaussian random variables $\boldsymbol{\Xi}_{\mathbf{k}}$ that satisfy the above constraint, we first generate independent and identically distributed Gaussian random variables $\boldsymbol{\Xi}'_{\mathbf{k}}$ and then linearly combine them to obtain random variables with the needed properties. For non-self-conjugate modes we use $\boldsymbol{\Xi}_{\mathbf{k}} = \frac{1}{\sqrt{2}}(\boldsymbol{\Xi}'_{\mathbf{k}} + \overline{\boldsymbol{\Xi}'_{\mathbf{N}-\mathbf{k}}})$ and for self-conjugate modes only the real-parts are non-zero with $\boldsymbol{\Xi}_{\mathbf{k}} = \frac{1}{2}(\boldsymbol{\Xi}'_{\mathbf{k}} + \overline{\boldsymbol{\Xi}'_{\mathbf{N}-\mathbf{k}}})$. For the deterministic forcing terms in the Magnus expansions, we use the approximation

$$\int_{t_n}^{t_{n+1}} \exp\left(\Omega_{\mathbf{k}}(t_{n+1}, s)\right) \hat{f}_{\mathbf{k}}(s) ds \approx \exp\left(\Omega_{\mathbf{k}}\left(t_{n+1}, \frac{t_n + t_{n+1}}{2}\right)\right) \int_{t_n}^{t_{n+1}} \hat{f}_{\mathbf{k}}(s) ds. \tag{40}$$

To compare our methods, we performed simulations of 10^8 trajectories and computed the relative error of the mean and covariance of the process at the final time, see Figure 7.

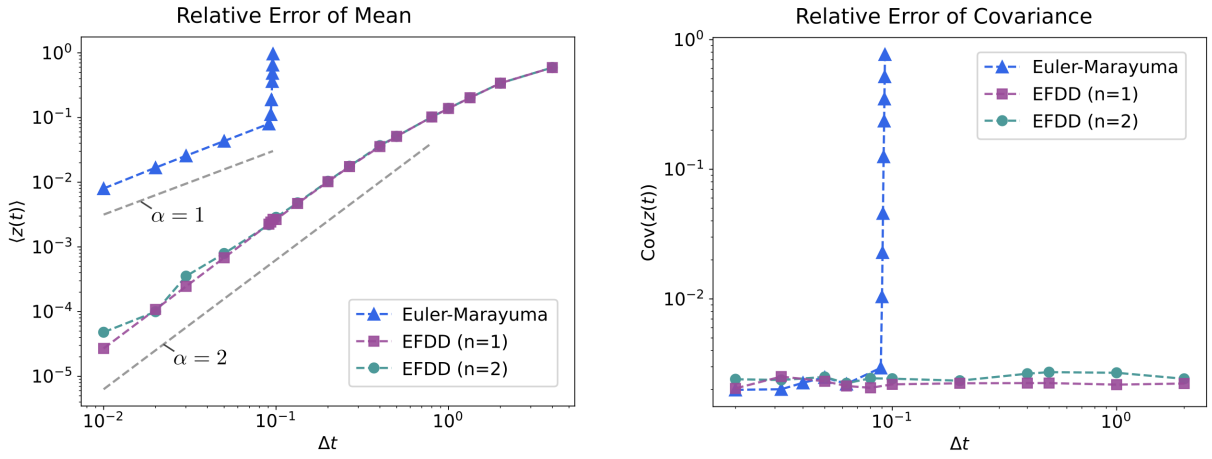

Figure 7: ***Accuracy of Methods.*** *We compare our stochastic magnus exponential integrator methods with Euler-Marayuma methods [29] for the SPDE in equation 33. The parameter values are* $D = 100$, $L = 100$, $N = 15$, $X(t) = L\sin(\omega t)$, $\omega = 1$, $c = 0.02$, $t_f = 4$, *and* $\hat{w}_{\mathbf{k}}(0) = 1$.

We find that the Euler-Maruyama Method exhibits a first-order accuracy with errors $O(\Delta t^{\alpha})$ with $\alpha = 1$. Our stochastic EFDDs with both $n = 1$ and $n = 2$ are found to exhibit second-order accuracy $\alpha = 2$. Given that the exponentials of the dissipative linear operator are diagonalizable in

the Fourier space, we find for both $n = 1$ and $n = 2$ that the primary error is from the approximation of the forcing term in equation 40. This yields comperable overall error for both EFDD methods. The Euler-Maruyama Method is found to be unstable when approaching magnitude $2/|\lambda|$ where λ is the eigenvalue largest in magnitude of $L(t)$ out of all t values in the simulation. For the chosen parameters, this value of Δt is approximately 7.4×10^{-2} with $\log(\Delta t) = -2.6$. In contrast to Euler-Maruyama, we find for our stochastic EFDD that even for larger Δ we are able to maintain accurate and stable results. This holds for another order of magnitude of time-steps.

Our EFDD approaches provide natural methods for discretizing such SPDEs both in space and time. In physical simulations, we need to ensure fluctuations contribute and propagate appropriately despite artifacts arising from the discretization errors. A further challenge in spatially extended systems is temporal stiffness that arises from disparities in time-scales associated with the different spatial scales resolved. For example, in our Fourier representation of the Laplacian $L(t)$ the scaling of the eigenvalues is $O(k^2)$ in the wavenumber k. In temporal finite difference methods, this can result in stiffness greatly limiting the time-steps required to maintain stability. More generally, the range of dynamic time-scales for relaxation in the system are closely related to the condition number of $L(t)$. Provided the operator $L(t)$ can be exponentiated efficiently our EFDD methods provide ways to overcome this stiffness allowing for stable time-step integration over long time-steps. Our EFDD methods also maintain fluctuation-dissipation balance which preserves statistical structures of the dynamics. The EFDDs we have presented here also can be used more generally to build stable long-time integrators for related dissipative SPDEs.

5 Conclusions

We have developed stochastic exponential time-step integrators for SPDEs and SDEs with stiff dynamics, referred to as Exponential Fluctuation-Dissipation Discretizations (EFDDs). Our EFDDs provide methods for avoiding the need to evaluate directly iterated stochastic integrals. The EFDD methods preserve statistical structures of the dynamics associated with fluctuation dissipation balance. When discretizing in space and time, our EFDD approach takes into account artifacts of the discretization errors to help ensure consistency between the discrete dissipative operators and approximations used for the stochastic terms. This helps to ensure appropriate propagation of fluctuations. We demonstrated our methods for SDEs and SPDEs with time-varying dissipative operators. Our results show for time-varying stochastic systems the EFDD methods are capable of yielding both higher-order accuracy and stability over long time-scales. The EFDD approaches provide practical ways to build stable long-time exponential integrators for time-varying dissipative stochastic systems.

6 Acknowledgements

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