AN EFFICIENT DATA-DRIVEN SOLVER FOR FOKKER-PLANCK EQUATIONS: ALGORITHM AND ANALYSIS.

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Abstract. Computing the invariant probability measure of a randomly perturbed dynamical system usually means solving the stationary Fokker-Planck equation. This paper studies several key properties of a novel data-driven solver for low-dimensional Fokker-Planck equations proposed in [15]. Based on these results, we propose a new “block solver” for the stationary Fokker-Planck equation, which significantly improves the performance of the original algorithm. Some possible ways of reducing numerical artifacts caused by the block solver are discussed and tested with examples.

1. Introduction

Random perturbations to deterministic dynamical systems are ubiquitous in models used in physics, biology and engineering. The steady state of a randomly perturbed dynamical system is of critical interest in the study of these physical, biological or chemical systems and their applications. From a dynamical systems point of view, the interplay of dynamics and noise is both interesting and challenging, especially if the underlying dynamics is chaotic. Characteristics of the steady state distribution also help us to understand asymptotic effects of random perturbations to deterministic dynamics.

The evolution of the probability density function of a randomly perturbed system is described by the Fokker-Planck equation [21]. Consider a stochastic dynamical system

\begin{equation}
\mathrm{d}X_t = f(X_t) \mathrm{d}t + \sigma(X_t) \mathrm{d}W_t, \tag{1.1}
\end{equation}

where \( f \) is a vector field in \( \mathbb{R}^n \), \( \sigma \) is a coefficient matrix, and \( \mathrm{d}W_t \) is an \( n \)-dimensional white noise. The corresponding Fokker-Planck equation, which is also known as the Kolmogorov forward equation, is

\begin{equation}
\frac{\partial u}{\partial t} = \mathcal{L} u = - \sum_{i=1}^{n} (f_i u)_x + \frac{1}{2} \sum_{i,j=1}^{n} (D_{ij} u)_{x,x}, \tag{1.2}
\end{equation}

where \( D = \sigma^T \sigma \), \( u(x,t) \) denotes the probability density at time \( t \), and subscripts \( t \) and \( x_i \) denote partial derivatives. In this paper, we focus on the invariant probability measure of (1.1), whose density function satisfies the stationary Fokker-Planck equation.

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equation

\[ \mathcal{L}u = 0 \quad \int_{\Omega} u \, dx = 1. \]

Detailed assumptions about equation (1.1) and (1.2) will be given in Section 2.1.

For Langevin dynamics, the invariant probability measure is given by the Gibbs distribution which can be computed up to the unknown normalizing constant; however, in general, the Fokker-Planck equation can not be solved analytically. Rigorous estimations of the invariant probability density function are challenging as well. Most known results are proved by large deviations techniques [8], which unfortunately only shows tail properties when the noise is asymptotically small. Some concentration properties of the invariant probability measure can be proved by assuming some dissipative conditions. For example, it was shown in [16] that such concentration in the vicinity of a strong attractor is “Gaussian-like”. However, these theoretical results can rarely give a satisfactory quantitative description of the invariant probability measure. Therefore, numerical solution techniques are necessary to further study these randomly perturbed dynamical systems. Numerically solving a steady state Fokker-Planck equation in an unbounded domain is nontrivial. And additional challenges are presented in systems with high dimensionality, chaotic underlying dynamics, and multiscale coefficient terms.

One difficulty of solving the Fokker-Planck equation numerically is the conflict between the need for high-resolution local solutions and the necessity to handle large spatial domains. On one hand, in many applications, what we need is a high-resolution local numerical solution. It is known that the invariant probability measure tends to concentrate at the vicinity of the global attractor, and for such systems we are interested in the distribution in a local region of the phase space. In addition, if the strength of noise \( \sigma \) is small, it is proved that the probability density function is concentrated in an \( O(\sigma) \) neighborhoods of the global attractor [16]. So in order to obtain a meaningful solution and to avoid numerical artifacts, the grid size needs to be small enough. On the other hand, the Fokker-Planck equation in \( \mathbb{R}^d \) is defined on an unbounded domain with zero value at infinity. The lack of a local boundary condition makes the problem computationally challenging. The existing methods usually solve the Fokker-Planck equation in a region that is large enough to cover all attractors.

In [15], a hybrid method is proposed to partially resolve the difficulties. The method deals with the local Fokker-Planck equation and completely removes the unknown boundary condition, which makes the resultant linear system undetermined. To solve this underdetermined problem, Monte-Carlo simulation is used to provide a reference solution for the numerical solver (finite difference or finite element). The reference solution itself has low accuracy and lots of undesired fluctuations. The algorithm then projects the “noisy” reference solution onto the kernel of the discretized numerical solver. This minimizes the distance between the collection of possible numerical solutions (without knowing the boundary condition) and the reference solution from the Monte Carlo simulation. This method can solve the problem in any local area even if it doesn’t cover any attractor. It also smooths the
oscillation caused by the Monte Carlo sampling. By reducing the computational cost from non-locality, it can provide a high resolution solution in a local area.

Paper [15] only introduced the algorithm without proof. Analysis of this algorithm is carried out in this paper. We proved that the hybrid method introduced in [15] can significantly reduce the error of the reference solution produced by the Monte Carlo simulation. The heuristic reason is that the error term of this random reference solution is very close to an i.i.d. random vector. The expected norm of this random vector is dramatically reduced when projecting it to a lower dimensional subspace. In addition, we use a combination of rigorous analysis and numerical computations to show that the error term of this projection concentrates on the boundary of the numerical domain. In other words, the empirical performance of the hybrid algorithm is actually much better than what can be rigorously proved.

The other goal of this paper is to improve the performance of this hybrid method by introducing block solvers. This improvement is motivated by the locality of the hybrid method. Since the hybrid method does not rely on local boundary conditions, we can divide the numerical domain into a large number of small blocks and apply the hybrid method to each block. The global solution is a collage of local solutions on these blocks. This divide-and-conquer strategy is very efficient. Consider a $d$-dimensional problems with $N$ grid points in each dimension. The classical numerical PDE solver needs to solve a large linear system with $N^d$ variables. Assume the cost of solving a linear system with $n$ variables is $O(n^p)$. Then the total cost is $O(N^{dp})$, which is considerably large if for instance $d = 3$ and $N = 1000$. However, if we divide the grid into many blocks with only $m$ grid points in each dimension. The total cost of solving the Fokker-Planck equation on $(N/m)^d$ blocks becomes $m^{pd} \times (N/m)^d = m^{(p-1)d}N^d$. Empirically $m$ can be as small as $20 – 30$. This dramatically reduces the total computational cost, unless the linear solver can achieve a linear complexity (which usually does not happen). In addition, parallelizing these block solvers is much easier than computing a large linear system in parallel. Instead of a local solution in a small subset of the phase space demonstrated in [15], the block solver now allows us to compute the full invariant probability density function of 3D or 4D systems, as demonstrated later in this paper.

The idea of using local blocks is supported by our analytical results in the first half of this paper. Theoretically, using larger blocks gives better reduction of error terms from Monte Carlo simulations, as proved in Theorem [21]. But the analysis in this paper shows that the error tends to concentrate at the boundary of blocks. Hence the size of blocks needs not to be very large to make the accuracy of solutions in the interior of blocks acceptable. And the error on the boundary can be repaired by algorithms. Since the error of numerical solution mainly concentrates on the boundary, a naive block solver has visible interface errors between blocks. We then develop methods to reduce this interface error. Two different approaches, namely the overlapping blocks method and the shifting blocks method, are introduced and tested with several examples.

In this paper, we mainly consider low-dimensional systems up to dimension 3 or 4, where traditional grid-based numerical methods still work. For systems in much
higher dimensions, all traditional grid-based methods of solving the Fokker-Planck equation, such as finite difference method or finite elements method, are not feasible any more. Direct Monte Carlo simulation also greatly suffers from the curse-of-dimensionality. There are several techniques introduced to deal with certain multi-dimensional Fokker-Planck equations, such as the truncated asymptotic expansion, splitting method, orthogonal functions, and tensor decompositions \[6, 7, 17, 23, 22\]. In particular, \[2, 3\] introduced an efficient technique for a class of high-dimensional dynamical systems. In the future, we will incorporate these high-dimensional sampling techniques to the mesh-free version of this hybrid algorithm.

The rest of this paper is organized as follows. In Section 2 we review the hybrid method in \[15\] and rigorously analyze the convergence of the method. We also show that the error will concentrate on the boundary of the domain. A directed block solver is proposed in Section 3. Two possible methods to repair interface error between blocks are studied in Section 4. In Section 5, we use three example systems to test our algorithms and error reduction methods. Section 6 is the conclusion.

2. Analysis of data-driven Fokker-Planck solver

2.1. Algorithm description. Consider a stochastic differential equation

\[
\frac{dX_t}{dt} = f(X_t)dt + \sigma(X_t)dW_t,
\]

where \(X_t \in \mathbb{R}^n\), \(f : \mathbb{R}^n \to \mathbb{R}^n\) is a continuous vector field, \(\sigma\) is a \(n \times n\) matrix-valued function, and \(dW_t\) is the white noise in \(\mathbb{R}^n\). We assume that \(f\) and \(\sigma\) has enough regularity such that equation (2.1) admits a unique solution \(X_t\) that is a Markov process with a transition kernel \(P^t(x, \cdot)\). Similar as in \[15\], we further assume that \(X_t\) admits a unique invariant probability measure \(\pi\) such that

\[
\pi P^t(A) = \int_{\mathbb{R}^n} P^t(x, A)\pi(dx)
\]

for any measurable set \(A\). In addition, we assume \(\pi\) is absolutely continuous with respect to the Lebesgue measure, and \(P^t(x, \cdot)\) converges to \(\pi\) for any \(x \in \mathbb{R}^n\). We refer \[20, 12, 24, 1, 11, 13, 19, 10\] for the detailed conditions that lead to the existence of solutions of (2.1), the existence of an invariant probability measure, and the convergence to the invariant probability measure.

Let \(u\) be the probability density function of \(\pi\). It is well known that \(u\) satisfies the stationary Fokker-Planck equation

\[
0 = \mathcal{L}u = -\sum_{i=1}^{n} (f_i u)_{x_i} + \frac{1}{2} \sum_{i,j=1}^{n} (D_{ij} u)_{x_i x_j},
\]

where \(D = \sigma^T \sigma\). In addition, because of the convergence, we have

\[
u(x) = \lim_{T \to \infty} \frac{1}{T} \int_0^T u(x, t) dt,
\]

where \(u(x, t)\) is the probability density function of \(X_t\).

For the sake of simplicity we assume \(n = 2\) when introducing the algorithm. But our algorithm works for any dimension. Now assume that we would like to solve
u numerically on a 2D domain \( D = [a_0, b_0] \times [a_1, b_1] \). To do this, an \( N \times M \) grid is constructed on \( D \) with grid size \( h = (b_0 - a_0)/N = (b_1 - a_1)/M \). Since \( u \) is the density function, we approximate it at the center of each of the \( N \times M \) boxes \( \{ O_{i,j} \}_{i=1}^{N,M} \) with \( O_{i,j} = [a_0 + (i-1)h, a_0 + ih] \times [a_1 + (j-1)h, a_1 + jh] \). Let \( u = \{ u_{i,j} \}_{i=1}^{N,M} \) be this numerical solution on \( D \) that we are interested in. 

\[
Au = 0, 
\]

where \( A \) is an \((N-2)(M-2) \times (NM)\) matrix. \( A \) is said to be the discretized Fokker-Planck operator.

Then we need the Monte Carlo simulation to produce a reference solution. Let \( \{ X_n \}_{n=1}^{N} \) be a long numerical trajectory of the time-\( \delta \) sample chain of \( X_t \), i.e., \( X_n = X_{n\delta} \), where \( \delta > 0 \) is the time step size of the Monte Carlo simulation. Let \( v = \{ v_{i,j} \}_{i=1,j=1}^{N,M} \) such that

\[
v_{i,j} = \frac{1}{Nh^2} \sum_{n=1}^{N} 1_{O_{i,j}}(X_n).
\]

It follows from the ergodicity of (2.1) that \( v \) is an approximate solution of (2.2). Again, we denote the \( N \times M \) vector reshaped from \( v \) by \( v \) as well.

As introduced in [15], we look for the solution of the following optimization problem

\[
\begin{align*}
(2.3) & \quad \min \| u - v \|_2 \\
& \text{subject to } Au = 0.
\end{align*}
\]

This is called the least norm problem. Vector

\[
(2.4) \quad u = A^T(AA^T)^{-1}(-Av) + v
\]

solves the optimization problem (2.3).

2.2. Error analysis through projections. The aim of this section is to show that the solution \( u \) to the optimization problem (2.3) is a good approximation of the global analytical solution \( u \) on \( \mathbb{R}^2 \). Let \( u^{\text{ext}} = \{ u_{i,j}^{\text{ext}} \} = u(ih + a_0 - h/2, jh + a_1 - h/2) \) be the values of the exact solution \( u \) at the centres of the boxes. We assume that the Monte Carlo simulation produces an unbiased sample \( v \) that approximates \( u^{\text{ext}} \). We note that this assumption is usually not exactly satisfied because the invariant probability measure of the numerical scheme that produces \( \{ X_n \} \) is only an approximation of \( \pi \). We refer [14] for known results about the difference between
the two invariant measures for Langevin dynamics and \cite{18} for that of generic stochastic differential equations. However, when $N$ is large (at least $10^7 \sim 10^8$ in our simulations), $v - u^{\text{ext}}$ is usually “noisy” enough to be treated as a vector of i.i.d. random numbers. Improving the quality of sampling is extremely important to this algorithm. We will address sampling methods in our subsequent work.

In order to make the rigorous proof, we need the following assumption.

(H)

(a) For $i = 1, \ldots, N, j = 1, \ldots, M$, $v_{i,j} - u_{i,j}^{\text{ext}}$ are i.i.d random variables with expectation 0 and variance $\zeta^2$.

(b) The finite difference scheme for equation (2.2) is convergent for the boundary value problem on $[a_0, b_0] \times [a_1, b_1]$ with $L^\infty$ error $O(h^p)$.

The performance of the algorithm is measured by $h \mathbb{E}[\|u - u^{\text{ext}}\|^2]$, which is the $L^2$ numerical integration of the error term. Before solving the optimization problem (2.3), we have $h \mathbb{E}[\|v - u^{\text{ext}}\|^2] = O(\zeta h N) = O(\zeta)$.

**Theorem 2.1.** Assume (H) holds. We have the following bound for the $L^2$ error $h \mathbb{E}[\|u - u^{\text{ext}}\|^2] \leq O(h^{1/2} \zeta) + O(h^p)$.

**Proof.** In order to proceed, we need an auxiliary vector that satisfies the linear constraint in equation (2.3). Consider the Fokker-Planck equation on the extended domain $\tilde{D} = [a_0 - h, b_0 + h] \times [a_1 - h, b_1 + h]$ with boundary condition

\[
\begin{aligned}
\mathcal{L}w &= 0 & & (x, y) \in \tilde{D} \\
w(x, y) &= u(x, y) & & (x, y) \in \partial \tilde{D},
\end{aligned}
\]

where $h$ is the mesh size. This problem is well-posed and has a unique solution $u(x, y), (x, y) \in \tilde{D}$.

Consider the discretization of (2.5) by finite difference method. It is of the following form

\[
\begin{bmatrix}
A & 0 \\
B & C
\end{bmatrix}
\begin{bmatrix}
u_{\text{lin}} \\
u_0
\end{bmatrix}
= \begin{bmatrix}
0 \\
0
\end{bmatrix},
\]

where the extended equations

\[
\begin{bmatrix}
B & C
\end{bmatrix}
\begin{bmatrix}
u_{\text{lin}} \\
u_0
\end{bmatrix}
= 0
\]

are the equations for the variables on the boundary $\partial D$ of $D$, and $u_0$ are the values of $u(x, y)$ at grid points on the boundary $\partial \tilde{D}$ of $\tilde{D}$. This boundary value problem gives a solution $u_{\text{lin}}$ that satisfies the linear constraint. By assumption (H), we have

\[\|u_{\text{lin}} - u^{\text{ext}}\|_\infty = O(h^p).\]

By the triangle inequality, it is sufficient to estimate

\[\|u - u_{\text{lin}}\|_2.\]

Let $P$ be the projection matrix to $\text{Ker}(A)$. Then equation (2.3) implies $u = P v$. Since $u_{\text{lin}} \in \text{Ker}(A)$, we have

\[u - u_{\text{lin}} = P v - u_{\text{lin}} = P(v - u_{\text{lin}}) = P(v - u^{\text{ext}}) + P(u^{\text{ext}} - u_{\text{lin}}).\]
Take the $L^2$ norm on both side and apply the triangle inequality, we have
\begin{equation}
 h\|u - u^{\text{lin}}\|_2 \leq h\|P(v - u^{\text{ext}})\|_2 + h\|P(u^{\text{ext}} - u^{\text{lin}})\|_2. 
\end{equation}

The second term is easy to bound because
\begin{equation}
 h\|P(u^{\text{ext}} - u^{\text{lin}})\|_2 \leq h\|u^{\text{ext}} - u^{\text{lin}}\|_2 
\leq hN\|u^{\text{ext}} - u^{\text{lin}}\|_\infty = O(h^p). 
\end{equation}

By assumption (H), $w = v - u^{\text{ext}}$ is a random vector with i.i.d. entries. And $P$ projects $w$ from $\mathbb{R}^{N \times N}$ to $\text{Ker}(A)$. Note that the dimension of $\text{Ker}(A)$ is $4N - 4$. Let $S \in SO(N^2)$ be an orthogonal matrix such that the first $4N - 4$ columns of $S^T$ form an orthonormal basis of $\text{Ker}(A)$. Let $s_1, \ldots, s_{4N-4}$ be column vectors of $S^T$. Then $S$ is a change-of-coordinate matrix such that $\text{Ker}(A)$ is spanned by $s_1, \ldots, s_{4N-4}$.

Let
\[ S\hat{w} = [\hat{w}_1, \ldots, \hat{w}_{4N^2}]^T. \]

We have
\[ PW = \sum_{i=1}^{4N-4} \hat{w}_i s_i. \]

This implies
\[ \mathbb{E}[\|PW\|_2] = \mathbb{E}\left[ \left( \sum_{i=1}^{4N-4} \hat{w}_i^2 \right)^{1/2} \right] \leq \left( \sum_{i=1}^{4N-4} \mathbb{E}[\hat{w}_i^2] \right)^{1/2}, \]

because $\{s_{i=1}^{4N^2}\}$ are orthonormal vectors.

We have
\[ \hat{w}_i = \sum_{j=1}^{N^2} S_{ji} w_i, \]

where $w_i$ is the $i$-th entry of $w$. $S$ is orthogonal hence
\[ \sum_{j=1}^{N^2} S_{ji}^2 = 1. \]

Recall that entries of $w$ are i.i.d. random variables with expectation zero and variance $\zeta^2$. This implies
\[ \mathbb{E}[\hat{w}_i^2] = \zeta^2 \sum_{j=1}^{N^2} S_{ji}^2 = \zeta^2. \]

Hence
\begin{equation}
 \mathbb{E}[\|v - u^{\text{ext}}\|_2] = \mathbb{E}[\|PW\|_2] \leq \sqrt{4N - 4} \cdot \zeta. 
\end{equation}

The proof is completed by combining equations (2.6), (2.7), and (2.8). \qed
2.3. Concentration of errors. The empirical performance of our algorithm is actually much better than the theoretical bound given in Theorem 2.1. This is because the error term $u - u^{\text{ext}}$ usually concentrates at the boundary of the domain. To see this, we can calculate the basis of $\text{Ker}(A)$. In 1D, $\text{Ker}(A)$ only contains two linear functions, which has very little error concentration. In 2D, for the case of the Laplacian, $f = 0$ on the unit square domain with $M = N$, a basis of $\text{Ker}(A)$ can be explicitly given. The following proposition follows easily from some elementary calculations.

**Proposition 2.2.** Let $A$ be the discretized Laplacian on a square domain with $N \times N$ grids. Without loss of generality assume $N$ is odd. Let $(x, y) = (\frac{i-1}{N-1}, \frac{j-1}{N-1})$ and $h = 1/(N - 1)$. Define vectors $u^{k,p} \in \mathbb{R}^{N \times N}, p = 1, \ldots, 8$ by

\[
\begin{align*}
    u_{i,j}^{k,1} &= b_k \sin(2k \pi x) e^{c_k y}, & u_{i,j}^{k,2} &= b_k^2 \cos(2k \pi x) e^{c_k y}, \\
    u_{i,j}^{k,3} &= b_k^3 \sin(2k \pi x) e^{c_k(1-y)}, & u_{i,j}^{k,4} &= b_k^4 \cos(2k \pi x) e^{c_k(1-y)}, \\
    u_{i,j}^{k,5} &= b_k^5 \sin(2k \pi y) e^{c_k x}, & u_{i,j}^{k,6} &= b_k^6 \cos(2k \pi y) e^{c_k x}, \\
    u_{i,j}^{k,7} &= b_k^7 \sin(2k \pi y) e^{c_k(1-x)}, & u_{i,j}^{k,8} &= b_k^8 \cos(2k \pi y) e^{c_k(1-x)},
\end{align*}
\]

where $c_k = h^{-1} \cosh^{-1}(2 - \cos(2k \pi h)), k = 1, \ldots, (N - 3)/2$ for $u^{1,1}, u^{1,3}, u^{1,5}, u^{1,7}$ and $k = 1, \ldots, (N - 1)/2$ for $u^{2,1}, u^{2,3}, u^{2,5}, u^{2,7}$, and $b_k^p$ are normalizers to make $\|u^{k,p}\|_2 = 1$. Further define vectors $\mathbf{u}^{l,p} \in \mathbb{R}^{N \times N}, p = 1, 2, 3, 4$ such that

\[
\begin{align*}
    u_{i,j}^{l,1} &= 1, & u_{i,j}^{l,2} &= x, & u_{i,j}^{l,3} &= y, & u_{i,j}^{l,4} &= xy.
\end{align*}
\]

Then

\[
\mathcal{B} = \{\{u^{k,p}\}_{p=1}^8, \{u^{l,p}\}_{p=1}^4\}
\]

is a basis of $\text{Ker}(A)$.

The basis $\mathcal{B}$ in Proposition 2.2 is nearly an orthonormal basis in most directions. For example, a QR decomposition of vectors in $\mathcal{B}$ shows that most diagonal terms nearly equal to 1 even for large $N$, as shown in Figure 1. The only exception is $u^{4,4}$, whose corresponding diagonal term is only 0.015. The exponential terms in vectors $u^{k,p}$ indicate exponential decay of the solution away from the boundary. Since $4N - 8$ out of $4N - 4$ vectors in $\mathcal{B}$ has significant concentration at the boundary, we expect the concentration of error at the boundary with a high probability.

The basis of $\text{Ker}(A)$ for the general case can not be explicitly given. Instead, we can compute principal angles between $\text{Ker}(A)$ and $\Theta_D$, where $\Theta_D$ is the subspace spanned by coordinate vectors corresponding to boundary layer with thickness $D$. In other words,

\[
\Theta_D = \text{span}\{e_{i,j} \mid i \leq D \text{ or } j \leq D \text{ or } i \geq N - D \text{ or } j \geq N - D\}.
\]

If most principal angles are small, $\text{Ker}(A)$ is almost parallel with $\Theta_D$. And the projection of a random vector to $\Theta_D$ preserves most of its length. In other words, we see a concentration of error terms at the boundary of the domain.
Figure 1. Diagonal entries from the $R$ matrix of the $QR$ decomposition of the basis $B$ in (2.9) and (2.10) respectively arranged in lexicographical order. The basis functions are nearly orthogonal. The mesh size $N$ is 101. Value of last diagonal entry is 0.015.

Principal angles $0 \leq \theta_1 \leq \cdots \leq \Theta_{4N-4} \leq \pi/2$ are a sequence of angles that describe the angle between $\text{Ker}(A)$ and $\Theta_D$. The first one is

$$\theta_1 = \min\{\arccos\left(\frac{\alpha \cdot \beta}{\|\alpha\|\|\beta\|}\right) \mid \alpha \in \text{Ker}(A), \beta \in \Theta_D\} = \angle(\alpha_1, \beta_1).$$

Other angles are defined recursively with

$$\theta_i = \min\{\arccos\left(\frac{\alpha \cdot \beta}{\|\alpha\|\|\beta\|}\right) \mid \alpha \in \text{Ker}(A), \beta \in \Theta_D, \alpha \perp \alpha_j, \beta \perp \beta_j, \forall 1 \leq j \leq i-1\},$$

such that $\angle(\alpha_i, \beta_i) = \theta_i$. Without loss of generality assume $\|\alpha_i\| = 1$ for all $1 \leq i \leq 4N-4$. Since $\dim(\Theta_D) \geq \dim(\text{Ker}(A))$, it is easy to see that $\{\alpha_1, \cdots, \alpha_{4N-4}\}$ forms an orthonormal basis of $\text{Ker}(A)$. Recall that $u \in \text{Ker}(A)$ and that the error $u - u^{\text{ext}}$ is approximated by the project of a random vector $w$ with i.i.d. entries to the subspace $\text{Ker}(A)$. Hence we can further assume that $\xi = u - u^{\text{ext}}$ is approximated by a random vector

$$\xi = \sum_{i=1}^{4N-4} c_i \alpha_i,$$

where $c_i$ are i.i.d. random variables with zero mean and variance $\zeta^2$. Define

$$p_D(\xi) = \frac{\mathbb{E}[\|P_{\Theta_D} \xi\|]}{\mathbb{E}[\|\xi\|]}$$

(2.11)
as the mean weight of $\xi$ projected on to the boundary layer, where $P_{e_D}$ is the projection matrix to $\Theta_D$. Assume $\xi$ satisfies equation (2.11). It is easy to see that

$$p_D(\xi) = \frac{1}{4N-4} \sum_{i=1}^{4N-4} \cos(\theta_i).$$

Therefore, $p_D(\xi)$ measures the degree of concentration of errors on the boundary layer with thickness $D$.

Principal angles can be numerically computed by an SVD decomposition. In Figure 2, we list all principal angles for $D = 1, 2, 3$. The matrices in Figure 2 are given by discretization of 2D Fokker-Planck equations (2.2) for $f = 0$ (left panel) and $f$ as in equation 5.1 (right panel). The size of a block is $(50 + D) \times (50 + D)$. We can see that the mean weight of $\xi$ projected to $\Theta_D$ is very large. In other words most of the error term $u - u^\text{ext}$ concentrates at the boundary layer. We also remark that the degree of concentration of error terms increases with the dimension.

The 2D case is demonstrated in Figure 2. And our computation shows that the error concentration is even more significant in 3D.

![Figure 2](image1.png)

**Figure 2.** Principal angles between Ker($A$) and $\Theta_D$ for $D = 1, 2, 3$. Left: Diffusion process without drift. Right: Fokker-Planck equation as given in Example 5.1.

Figure 3 shows an empirical test of the spatial distribution of error terms. The Fokker-Planck equation is still from the ring density function as in Section 5.1. We choose a $64 \times 64$ block on $[0, 1] \times [0, 1]$ and solve the Fokker-Planck equation with our hybrid solver. The Monte Carlo simulation uses $10^6$ sample points. The numerical solutions $v$ and $u$ are compared with the exact solution $u^\text{ext}$ in the top left and right panel, respectively. As a comparison, we also produce $10^6$ unbiased samples from the invariant density itself, denoted by $v'$. The solution of the hybrid solver from $v'$
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is denoted by \( u' \). We can clearly see that most error of \( u \) and \( u' \) concentrates at the boundary of the domain. The bottom panel compares the relative weight of error concentrating on the boundary layer for \( D = 1, 2, 3, 4 \). The relative weights \( \rho_u \) and \( \rho_v \) are given by

\[
\rho_u = \frac{\|P_{\mathcal{D}}(v - u^{\text{ext}})\|}{\|v - u^{\text{ext}}\|}, \quad \rho_v = \frac{\|P_{\mathcal{D}}(u - u^{\text{ext}})\|}{\|u - u^{\text{ext}}\|},
\]

respectively. \( \rho_{u'} \) and \( \rho_{v'} \) are also defined analogously.

From Figure 3, the spatial concentration of \( u - u^{\text{ext}} \) on the boundary layer is less than the theoretical prediction given before, mainly because the sample itself has bias. But we can still see a significant concentration of error on the boundary layer. The error concentration of \( u' - u^{\text{ext}} \) is much better. Almost all errors of \( u' \) are concentrated on the two boundary layers. It is worth to mention that although the unbiased sample \( v' \) has little visual difference from the Monte Carlo data \( v \), the resultant solution \( u' \) has significant better performance in terms of error concentration on the boundary. Hence this example also demonstrates the importance of choosing a good Monte Carlo sampler.

3. Block Fokker-Planck Solver

Since we can use the hybrid method to compute the Fokker-Planck equation on any region in the phase space, a straightforward improvement is to apply the divide-and-conquer strategy. We can divide the interested numerical domain into small blocks and then combine the results on these blocks to generate the solution on the original big domain. As discussed in the introduction, assume we divide an \( N^d \) mesh into many \( m^d \) blocks, where \( m \ll N \). If the linear solver to an \( n \times n \) matrix has \( O(n^p) \) complexity (usually \( p > 1 \)), the total computational cost is reduced from \( N^{pd} \) to \( m^{(p-1)d}N^d \). In addition, this block solver significantly simplifies parallel computing, since all blocks are independent and satisfy the same Fokker-Planck equation. We can also change the grid size for each block based on whether the data is dense or sparse in a subregion to further reduce the computational cost. Moreover, we can apply our method to problems with irregular domains by dividing it into many small rectangular blocks.

For simplicity, we still use a rectangular domain \( D = [a, a'] \times [b, b'] \) to describe our algorithm, and assume that we want to solve \( u \) in \( D \). We divide \( D \) into \( K \times L \) blocks \( \{D_{k,l}\}_{k=1,l=1}^{K,L} \) with \( D_{k,l} = [a_{k-1}, a_k] \times [b_{l-1}, b_l] \), where \( a_k = a + k(a' - a)/K \) and \( b_l = b + l(b' - b)/L \).

Following the algorithm presented in Section 2.1, we construct an \( N \times M \) grid on \( D_{k,l} \) and discretize the Fokker-Planck equation. This gives a linear constraint

\[
A_{k,l}u^{k,l} = 0
\]

on \( D_{k,l} \), where \( A_{k,l} \) is a \( (N-2)(M-2) \times (NM) \) matrix. Then we obtain a reference solution \( v^{k,l} \) from the Monte-Carlo simulation by picking up the corresponding values \( \{v^{k,l}_{i,j}\}_{i=1,j=1}^{N,M} \) from the global simulation result \( v \), such that

\[
v^{k,l}_{i,j} = v((k - 1)N + i, (l - 1)M + j)
\]
for $k = 1, \ldots, K, l = 1, \ldots, L, i = 1, \ldots, N, j = 1, \ldots, M$. This gives an optimization problem on $D_{k,l}$

$$
\min_{u} \|u - v_{k,l}\|_2 \\
\text{subject to} \quad A_{k,l}u = 0.
$$

(3.1)

We denote the solution to (3.1) by $u_{k,l}$, which can be obtained by calculating

$$
u_{k,l} = A_{k,l}^T (A_{k,l}A_{k,l}^T)^{-1}(-A_{k,l}v_{k,l}) + v_{k,l}.
$$

Now, the $(i,j)$ coordinate $u_{i,j}^{k,l}$ of $u_{k,l}$ is an approximation of $u$ at the point $(ih + a_{k-1} - h/2, jh + b_{l-1} - h/2)$, where $h = (a_k - a_{k-1})/N = (b_l - b_{l-1})/M$ is the grid size when we divide $D_{k,l}$ into $N \times M$ boxes. It remains to combine all local solutions $\{u_{k,l}\}_{k=1,l=1}^{K,L}$ on all blocks by collaging them together, i.e.,

$$
u(ih + a_{k-1} - h/2, jh + b_{l-1} - h/2) = u_{i,j}^{k,l}.
$$
The collage numerically solves the Fokker-Planck equation (2.2) on the whole domain $D$.

4. Reducing Interface Error

As discussed in Section 2.3, the optimization problem (2.3) projects most error terms to the boundary of the domain. For the block algorithm, the solution is less accurate near the boundary of each block. The error on the boundary usually looks noisy because it inherits the randomness from Monte Carlo simulations. As a result, there are visible fluctuations on the interface of two adjacent blocks. To make the block solver applicable, modifications to the solution on the interface of blocks are necessary.

In this section, we provide two different methods to reduce the interface error, i.e., the overlapping blocks method and the shifting blocks method. The overlapping blocks method expands each block locally, and keeps only the interior portion which has much lower observed errors. The shifting blocks method makes several smoothing passes, shifting the block boundaries each time so that portions previously on the edges are now in block interiors. Advantages and limitations of these methods will also be discussed.

4.1. Overlapping blocks. Since the numerical solution of the hybrid solver has much higher accuracy at interior points than on the boundary, the most natural approach is to discard the boundary layer. When applying the block solver, we can enlarge the blocks by one or two layers of boxes. Then we apply the algorithm in Section 2.1 on the enlarged block. The interior solution restricted to the original block is the new output of the block solver. This is called the overlapping blocks method.

More precisely, recall that we first divide $D = [a, a'] \times [b, b']$ into $K \times L$ blocks $\{D_{k,l}\}_{k=1,l=1}^{K,L}$, then divide each block $D_{k,l} = [a_{k-1}, a_k] \times [b_{l-1}, b_l]$ into $N \times M$ boxes $O_{i,j}^{k,l} = [a_{k-1} + (i - 1)h, a_{k-1} + ih] \times [b_{l-1} + (j - 1)h, b_{l-1} + jh]$, where $h = (a_k - a_{k-1})/N = (b_l - a_{l-1})/M$. Instead of $D$, now we work on the extended domain $\tilde{D}_{k,l} = [a - \iota h, a' + \iota h] \times [b - \iota h, b' + \iota h]$ of $D$.

Instead of disjoint blocks $D_{k,l}$, we construct an $(N + 2\iota) \times (M + 2\iota)$ grid on $\tilde{D}_{k,l}$ and generate the discretized Fokker-Planck equation

$$\tilde{A}_{k,l}^\iota u = 0$$

on $\tilde{D}_{k,l}$, where $\tilde{A}_{k,l}^\iota$ is a $(N + 2\iota - 2)(M + 2\iota - 2) \times ((N + 2\iota)(M + 2\iota))$ matrix. Then a local reference solution $\tilde{v}_{i,j}^{k,l}$ is obtained by picking up the corresponding value $v_{i,j}^{k,l}$ from the global simulation vector $\tilde{v}$. For each block, we solve the local optimization problem (3.1), and keep only the values at the interior points, $D_{k,l}$ to create the global approximation $u$.

The advantage of this overlapping block method is that it is very easy to implement. No additional treatment is necessary besides discarding one or two boundary
layers. But in higher dimension, a significant proportion of grid points will be on the boundary of blocks. For example, if \( t = 2 \), \( M = N = 30 \), the percentage of unused grid points is 13\% in 1D, 28\% in 2D, 46\% in 3D, and 65\% in 4D. Also, as seen in Figure 3, visible error inherited from the reference solution \( v \) can easily penetrate through 4 – 5 boundary layers. Hence the output of solutions from the overlapping block method usually still have some visible residual interface error.

4.2. Shifting blocks. The idea of shifting block is also motivated by the concentration of error of the solution of (2.3). To resolve the interface fluctuation between blocks, one can simply move the interface to the interior by shifting all blocks and recalculate the solution. Since the solution has much higher accuracy in the interior of a block, this can easily smooth the interface error. More precisely, after applying the block solver, we make a “half-block” shift of the blocks so that boundaries of the original blocks are now in the interior of new blocks. Then we solve optimization problems (2.3) again on newly shifted blocks. The reference solution fed into the optimization problem (2.3) is the numerical solution from the first round. If necessary, one can carry out this shifting block for several rounds to cover all grid points and to improve the accuracy.

Divide the domain \( D = [a, a'] \times [b, b'] \) into \( K \times L \) blocks \( \{D_{k,l}\}_{k=1}^{K} \times _{l=1}^{L} \) with \( D_{k,l} = [a_{k-1}, a_k] \times [b_{l-1}, b_l] \), where \( a_k = a + k(a' - a)/K \) and \( b_l = b + l(b' - b)/L \). Then we make half-block shifts to get the shifted blocks \( D'_{k,l} = [a'_{k-1}, a'_k] \times [b'_{l-1}, b'_l] \), where \( a'_k = a_k + (a' - a)/2K = a + (k + 1/2)(a' - a)/K \) and \( b'_l = b_l + (b' - b)/2L = b + (l + 1/2)(b' - b)/L \). The Monte Carlo data needs to cover all blocks \( D_{k,l} \) and \( D'_{k,l} \).

Now construct \( N \times M \) grids both on \( D_{k,l} \) and \( D'_{k,l} \), and generate the discretized Fokker-Planck equations

\[
A_{k,l} \mathbf{u} = \mathbf{0} \quad \text{and} \quad A'_{k,l} \mathbf{u} = \mathbf{0}
\]

on \( D_{k,l} \) and \( D'_{k,l} \) respectively, where \( A_{k,l} \) and \( A'_{k,l} \) are \((N - 2)(M - 2) \times (NM)\) matrices.

We first use the original block solver to solve the optimization problem on each \( D_{k,l} \), as described in Section 3. This gives approximated solutions \( \mathbf{u}_{k,l} \) on each block. The first approximation \( \mathbf{u}^1 \in \mathbb{R}^{MN} \) is obtained by collaging \( \mathbf{u}_{k,l} \) from all blocks.

Then we generate the reference solution \( \mathbf{v}^{k,l} \) on shifted blocks \( D'_{k,l} \) by using the corresponding values in \( \mathbf{u}^1 \) whenever available. More precisely we have

\[
\mathbf{v}^{k,l}_{i,j} = \mathbf{u}^1_{(k-1/2)N+i,(l-1/2)M+j}
\]

for \( k = 1, \ldots, K - 1, l = 1, \ldots, L - 1, i = 1, \ldots, N, j = 1, \ldots, M \). When \( k = K \) or \( l = L \), we use Monte Carlo data to produce \( \mathbf{v}^{k,l}_{i,j} \) if \( \mathbf{u}^1 \) data is not available. Then we solve the optimization problem (3.1) on the shifted block \( D'_{k,l} \) to get a numerical solution \( \mathbf{u}'_{k,l} \) on \( D'_{k,l} \).

Now \( \mathbf{u}'_{k,l} \) are computed on shifted blocks. We use data from \( \mathbf{u}'_{k,l} \) to produce the global solution whenever possible, that is, let

\[
u((k - 1)N + ih + a_{k-1} - h/2, (l - 1)M + jh + b_{l-1} - h/2) = u'_{i,j}
\]
for \( k = 2, \ldots, K, l = 2, \ldots, L, i = 1, \ldots, N, j = 1, \ldots, M \). If \( k = 1 \) or \( l = 1 \), we use values from \( u^1 \) if the data from \( u^r_{k,l} \) is not available.

We remark that in practice one does not have to shift the block by exactly one half. This shifting block method can be implemented repeatedly, such that the solution \( u' \) from last round is used as the reference solution for the next round. We find that one efficient way of implementation is to shift the block by \( 1/3 \) for two times to get two solutions \( u' \) and \( u'' \) on shifted blocks. Then we feed \( u'' \) back to the original block solver as the reference solution. This implementation covers all grid points by interiors of blocks. Using an iterative linear solver can significantly accelerate the shifting blocks method. Because from the second round, we have \( u_{k,l} \approx v_{k,l} \) at all interior grid points. Hence \( 0 \) is a good initial guess when solving \((A_{k,l}A_{k,l}^T)^{-1}(-A_{k,l}v_{k,l})\) in the optimization problem (3.1). Empirically, the total computation time of three shifts is roughly similar to the time needed for the first round, if the conjugated gradient linear solver is used.

5. Numerical Examples

In this section, we consider the following three numerical examples to test the performance of our methods.

5.1. Ring density function. Consider the following stochastic differential equation:

\[
\begin{align*}
    dx &= \left( -4x(x^2 + y^2 - 1) + y \right) dt + \varepsilon dW^x_t \\
    dy &= \left( -4y(x^2 + y^2 - 1) - x \right) dt + \varepsilon dW^y_t,
\end{align*}
\]

where \( W^x_t \) and \( W^y_t \) are independent Wiener processes. To compare the performance of different solvers in this paper, we fix the strength of white noise to be \( \varepsilon = 1 \). The deterministic part of equation (5.1) is a gradient system plus a perpendicular rotation term, where the potential function of the gradient component is

\[ V(x, y) = (x^2 + y^2 - 1)^2. \]
Figure 5. (Ring density) The approximation by Monte Carlo simulation (left) and the algorithm in Section 2.1 (right) with 256 × 256 mesh points and 10^7 samples.

See Figure 4 for selected trajectories of equation (5.1). The rotation term does not change the invariant probability density function. Therefore, the deterministic part of equation (5.1) admits a limit circle x^2 + y^2 = 1, and the invariant probability measure of (5.1) has density function

\[ u(x, y) = \frac{1}{K} e^{-2V/\varepsilon^2}, \]

where \( K = \pi \int_{-\infty}^{\infty} e^{-2t^2/\varepsilon^2} dt \) is the renormalization constant. Therefore, the stationary Fokker-Planck equation corresponding to (5.1) has an analytic global solution \( u(x, y) \) on \( \mathbb{R}^2 \) (Figure 4 Right).

We first look at the approximation obtained from Monte-Carlo simulation with 256 × 256 mesh points on the domain \( D = [-2, 2] \times [-2, 2] \), and use step size \( dt = 0.002 \) and 10^7 samples in the sampling step (the left figure in Figure 5). As expected, we can see that this approximation has too much fluctuation to be an acceptable solution of the stationary Fokker-Planck equation. But the algorithm in Section 2.1 provides a smoothed approximation of the exact solution (the right figure in Figure 5).

Then we test the performance of block solvers, which is the theme of the present paper. In addition, we need to compare the effect of two error reduction methods proposed in Section 4. In the next a few figures, we still use a 256 × 256 mesh on the domain \( D = [-2, 2] \times [-2, 2] \), and 10^7 samples to simulate the reference data \( \mathbf{v} \). We further divide \( D \) into 8 × 8 blocks, each of which thus has 32 × 32 mesh points. The left figure in Figure 6 is the approximation given by the naive block solver described in Section 3. As expected in Section 2.3 and explained at the beginning of Section 4, the error term of the Monte-Carlo simulation data \( \mathbf{v} \) (see Figure 5 (left)) is spread from the interior of each block to its boundary because of the projection, which causes visible interface fluctuation.

The next step is to implement two different error reduction methods introduced in Section 4 and compare their performances. The right of Figure 6 shows the solution
Figure 6. (Ring density) The approximation computed by the basic block solver (left) and 1-overlapping block solver (right) with $256 \times 256$ mesh points, $8 \times 8$ blocks and $10^7$ samples.

Figure 7. (Ring density) The approximation computed by a triple iterated half-block shifting solver (left) with $256 \times 256$ mesh points, $8 \times 8$ blocks and $10^7$ samples.

given by overlapping blocks with 1 layer of box overlap, that is, $\iota = 1$ (see Section 4.1). We can see that the interface fluctuation is reduced, especially at the places with high probability density function and high interface fluctuation. Figure 7 is obtained by iterating the shifting block solver (see Section 4.2) for three repeats. The interface fluctuation is not only reduced, but also smoothed significantly.

Here we compare numerical solutions of the invariant probability measure of equation (5.1), which is explicitly known. Figure 8 shows a comparison of error terms for solutions obtained by different error reduction methods, in both discrete $L^2(D)$ norm and discrete $H^1(D)$ norm. To make a fair comparison, we let the number of samples change with the grid size. Examples with mesh sizes $N = 64, 128, 256, 512, 1024,$ and 2048 are tested and compared. The block size is $32 \times 32$ in all tests. The total
number of Monte Carlo samples is chosen to be $390.625N^2$. From Figure 8, we can see that the $L^2$ error of the Monte Carlo data is stabilized as expected, because the average sample count per box (and per grid) is constant.

The performance of two error reduction methods are compared in Figure 8. We can see that the plain block solver reduces the error significantly compared to the Markov chain data, but the error does not seem to converge to zero. This is not a surprise because all blocks are $32 \times 32$, and Theorem 2.1 says that the error should be proportional to $-1/2$ power of the block size. Both error reduction methods reduces the $L^2$ error from the plain block solver to some degree. The shifting blocks method has better performance, but also a higher computational cost. We can see that the empirical rate of error decay for the shifting block method is roughly $N^{-1/2}$, which is better than the theoretical result in Theorem 2.1.

First order derivatives in the discrete $H^1(D)$ norm are calculated by taking finite differences with respect to nearest grid points. With a constant mean sample size per box, the $H^1(D)$ error of the reference solution from Monte Carlo data diverges when $N$ increases. This is because local fluctuations are roughly unchanged with the mesh size, while the grid size $h$ become smaller. Therefore, the derivative of the reference solution is $O(\zeta h^{-1})$, where $\zeta$ is the standard deviation of number of samples per box. In other words, all algorithms based on Monte Carlo simulations are expected to have poor performance in $H^1(D)$ error. The divergence of $H^1(D)$ error is alleviated by the overlapping block method, and partial overturned by the shifting blocks method. As we see in Figure 8 Right, when $N = 2048$, the shifting block method gives a solution whose $H^1(D)$ error is $>150$ times less than that of the Monte Carlo data.

We can see that due to the lack of interaction between blocks, the information of the reference solution obtained by the Monte-Carlo simulation is not transferred to a neighboring blocks. So if a block is over-sampled, while the others are under-sampled, then after the block solutions are pasted together, the graph is not “flat” at the places where it should be. We can see that the shifting block method has better performance in terms of improving the regularity. This is because it significantly increases interactions between the neighbourhood blocks, and transfers the information between neighborhood blocks. Applying the shifting block method repeatedly can make the result more close to the global solver or the exact solution. But it also incurs some extra computational cost, as seen in Table 1.

Finally, we show a comparison of computation time in Table 1. In Table 1, “Sampling” means the Monte Carlo sampling time (including a burn-in time, which is the waiting time before collecting samples). “Plain” means the plain block solver proposed in Section 3. “Overlapping” means overlapping blocks method with $\iota = 1$ in Section 4.1. “Shifting” means the shifting blocks method in Section 4.2. We shift blocks twice by $1/3$ and $2/3$, and feed the new solution to the original solver as the reference solution. And “Old Version” means the algorithm proposed in [15], where no block is used. To make a fair comparison, no parallelizations or iterative linear solvers are used in this performance testing. We can see that the Monte Carlo sampling actually takes most of the time, and all versions of block-based solvers are
very fast. When the mesh size is 2048, the plain block solver is > 100 times faster than solving a large optimization problem \((2.3)\) without dividing the domain.

| Mesh | Sampling | Plain | Overlapping | Shifting | Old Version |
|------|----------|-------|-------------|----------|-------------|
| 64   | 0.5697   | 0.007316 | 0.009327 | 0.022512 | 0.017317 |
| 128  | 1.21302  | 0.026459 | 0.037354 | 0.109024 | 0.124361 |
| 256  | 3.73153 | 0.11852 | 0.159628 | 0.483537 | 0.8035 |
| 512  | 14.1032 | 0.416178 | 0.601545 | 1.92014 | 10.9225 |
| 1024 | 57.606 | 1.87628 | 2.56352 | 7.83214 | 61.5952 |
| 2048 | 319.075 | 6.5266 | 9.04282 | 31.7321 | 781.52 |

Table 1: CPU time (in seconds) for different algorithms and mesh sizes.

5.2. Chaotic attractor. In this subsection, we apply our solver to a non-trivial 3D example. Consider the Rossler oscillator with a small random perturbations

\[
\begin{aligned}
    dx &= (-y - z) \, dt + \varepsilon \, dW_t^x \\
    dy &= (x + ay) \, dt + \varepsilon \, dW_t^y \\
    dz &= (b + z(x - c)) \, dt + \varepsilon \, dW_t^z,
\end{aligned}
\]
Figure 9. (Rossler) A trajectory in the Rossler system (5.2) (left) and its projection on the $xy$-plane (right).

where $a = 0.2$, $b = 0.2$, $c = 5.7$, $\varepsilon = 0.1$, and $W_t^x$, $W_t^y$, and $W_t^z$ are independent Wiener processes. This system is a representative example of chaotic ODE systems appearing in many applications of physics, biology and engineering. Figure 9 shows a trajectory in the corresponding deterministic system and its projection onto the $xy$-plane.

It is natural to imagine that the invariant density of (5.2) has a similar shape to Figure 9. We use the block solver together with 3 repetitions of the shifting blocks method on $D = [-15, 15] \times [-15, 15] \times [-1.5, 1.5]$ with $1024 \times 1024 \times 128$ mesh points. The grid is further divided into $32 \times 32 \times 4$ blocks. The reference solution is generated by a Monte Carlo simulation with $3.2 \times 10^{10}$ samples. Four “slices” of the solution, as seen in Figure 10, are then projected to the $xy$-plane for the sake of easier demonstration. Projection of the whole solution to the $xy$-plane is shown in Figure 11. In addition to the expected similar shape of the distribution, we can see that many fine local structures of the deterministic system are preserved by the invariant probability measure.

To demonstrate the performance of our algorithm, we apply the data-driven solver without blocks to three local regions with different characteristics (see Figure 11). In each region, we use the data-driven solver on $128 \times 128 \times 128$ mesh points without dividing the domain into blocks.

In Region I, $[-15/4, 0] \times [-15/8, 15/8]$, the projection of the solution has both dense and sparse parts that are clearly divided. In the first figure of 12, we can see that a similar resolution is preserved when using much smaller block sizes. Both solutions provide high resolution to demonstrate the influence of strong chaos on the invariant distribution. The only difference is the local solver with smaller blocks has higher error on the left and bottom boundary, because the half-shift method does not touch this part. The discrete $L^2$ norm of the difference between the restriction of global solution on Region I and the local solution is $\varepsilon_1 \approx 0.0032$. In Region II, $[-15/8, 15/8] \times [165/32, 285/32]$, the solution includes an outer “ring” with high density. Outside this “ring”, the density function decays quickly. We can see that
Figure 10. (Rossler) Projections of 4 “slices” of the invariant density of the Rossler system \([5,2]\) to the \(xy\)-plane. \(z\)-coordinates of 4 slices are \([-0.09375, 0.02344], [0.02344, 0.1406], [0.1406, 0.2578],\) and \([0.2578, 0.375]\). The solution is obtained by a half-block shift solver on \([-15, 15] \times [-15, 15] \times [-1.5, 2.25]\) with \(1024 \times 1024 \times 128\) mesh points, \(32 \times 32 \times 4\) blocks, and \(3.2 \times 10^{10}\) samples.

Both solutions show the decay of the density around this ring. The discrete \(L^2\) norm of this difference between the two solutions in Region II is \(\varepsilon_{II} \approx 0.0028\). In Region III, \([75/16, 135/16] \times [-45/4, 15/2]\), the local solution has much lower density. The local solver is still accurate when the entries of \(v\) are much smaller. The discrete \(L^2\) norm of the difference between the global solution and the local solution in this region is \(\varepsilon_{III} \approx 0.0018\).

Overall, the solution from the block solver has little difference from the one obtained over a large mesh. And the solver can provide desired resolution in both settings. Empirically, we find that a block size of \(30 - 35\) is a good balance of performance and accuracy for most 2D and 3D problems.
Figure 11. (Rossler) The projection of the whole solution of the Rossler system (5.2) to the $xy$-plane. Three different local regions I–III (the red boxes) are used for comparing block solvers with different block sizes. See Figure 12 also.

Figure 12. (Rossler) The local restrictions of the global solution in Region I–III (the first row), and the projections onto the $xy$-plane of solutions by the local solver in the three local regions (the second row).
5.3. Mixed mode oscillation. In this example, we consider another non-trivial 3D system of mixed mode oscillation (MMO) with small random perturbations

\[
\begin{align*}
\frac{dx}{\eta} &= \frac{1}{\eta}(y - x^2 - x^3) \, dt + \varepsilon \, dW^x_t \\
\frac{dy}{\eta} &= (z - x) \, dt + \varepsilon \, dW^y_t \\
\frac{dz}{\eta} &= (-\nu - ax - by - cz) \, dt + \varepsilon \, dW^z_t,
\end{align*}
\]

(5.3)

where \( \eta = 0.01 \), \( \nu = 0.0072168 \), \( a = -0.3872 \), \( b = -0.3251 \), \( c = 1.17 \), and \( W_t^x, W_t^y \) and \( W_t^z \) are independent Wiener processes. The strength of noise is chosen to be \( \varepsilon = 0.1 \). Figure 13 provides one trajectory of the corresponding deterministic system and its projection on the \( xy \)-plane. The deterministic part of equation (5.3) has a critical manifold \( y = x^2 + x^3 \), at which the derivative of the fast variable vanishes. We can see that oscillations with different amplitudes occur near the fold of the critical manifold, where the attracting and repelling sheet of the critical manifold meet. This is called the mixed mode oscillation (MMO) [5]. The mechanism of mixed mode oscillations is similar as that of the canard explosion, which means the trajectory can follow the unstable sheet of the critical manifold for some time [9]. It was observed in [15] that the canard explosion can be destroyed by a small random perturbation. This motivates us to explore the characteristics of MMO under random perturbations.

We again use the half-block shift solver with \( 2048 \times 512 \times 256 \) mesh points, \( 64 \times 16 \times 8 \) blocks and \( 10^9 \) samples to get the invariant measure on \( D = [-1.5, 0.5] \times [-0.15, 0.35] \times [-0.05, 0.05] \). The numerical result is still projected to the \( xy \)-plane (see Figure 14). We can see that the invariant measure is mainly supported by the neighborhood of the stable sheets of the critical manifold. Deterministic oscillations with small amplitude are eliminated by the random perturbation. In other words, similar to the canard explosion, MMO can not survive a small random perturbation. The mechanism of this phenomenon is still not clear. It is also not known how small the noise should be in order to see MMO in equation (5.3).

To corroborate the performance of the solver on local regions, in this example, we apply it to four ‘\( z \)-layers’, that is, the region in the phase space of the form \([-1.5, 0.5] \times [-0.15, 0.35] \times I \), where \( I = [-0.1, -0.1 + d], [-0.05, -0.05 + d], [0.05, 0.05 + d], \) and \([0.1, 0.1 + d]\) respectively with \( d = 1/32 \). In each layer, we apply an iterated shifting blocks solver with \( 2048 \times 512 \times 32 \) mesh points, \( 64 \times 16 \times 1 \) blocks, and \( 10^9 \) samples.

Figure 15 shows the invariant distribution in these four local layers when projected to the \( xy \)-plane. We can see the invariant density function on each \( z \)-layer. Similar as in Figure 14, most invariant density concentrates at two stable sheets of the invariant manifold, and no small amplitude oscillations can be seen from the invariant probability density function.

6. Conclusion

A hybrid method for computing the invariant probability measure of the Fokker-Planck equation was proposed in [15]. The key idea is to generate a reference solution from Monte Carlo simulation to partially replace the role of boundary conditions.
Figure 13. (MMO) A trajectory in the system of mixed mode oscillation (5.3) (left) and its projection on the $xy$-plane (right).

Figure 14. (MMO) The projection of the invariant density of the system (5.3) of mixed mode oscillation onto the $xy$-plane by a half-block shift solver on $[-1.5, 0.5] \times [-0.15, 0.35] \times [-0.1, 0.15]$ with $2048 \times 512 \times 256$ mesh points, $32 \times 32 \times 32$ blocks and $10^9$ samples.

In this paper, we rigorously proved the convergence of this hybrid method. The concentration of error is also investigated analytically and numerically. We found that the error tends to concentrate on the boundary of the numerical domain, which makes the empirical performance much better than our theoretical result. Motivated by these results and the divide-and-conquer strategy, we proposed a block version of this hybrid method. It dramatically reduces the computational cost for problems up to dimension 4. This method makes the computation of invariant probability measures possible for many stochastic differential equations arising in different fields, especially for researchers with limited computing resources. Finally, to repair the
Figure 15. (MMO) The projections onto the $xy$-plane of solutions by the local solver in the four $z$-layers).

interface error appearing at the interface between adjacent blocks, two different methods are proposed and tested with several numerical examples.

The block solver studied in this paper can be extended into several directions. A natural extension is the time-dependent Fokker-Planck equations. As discussed in [15], one only needs to slightly modify the optimization problem (2.3) to solve a time-dependent Fokker-Planck equation. This data-driven framework also works for other PDEs with available data from stochastic simulations, such as reaction-diffusion equations. It is well known that a chemical reaction system with diffusions can be computed by both the stochastic simulation algorithm (SSA) and the reaction-diffusion equation. This is similar to the case of the Fokker-Planck equation. In addition, mesh-free version of this block solver can be developed to solve higher dimensional problems. Some high-dimensional sampling methods [2, 3] can be adopted to improve the quality of sampling.

References

[1] V. Bogachev and M. Röckner, *A generalization of Khasminskii’s theorem on the existence of invariant measures for locally integrable drifts*, Theory of Probability and its Applications 45 (2001), 363.
[2] Nan Chen and Andrew J Majda, *Beating the curse of dimension with accurate statistics for the Fokker-Planck equation in complex turbulent systems*, Proceedings of the National Academy of Sciences **114** (2017), no. 49, 12864–12869.

[3] ______, *Efficient statistically accurate algorithms for the Fokker-Planck equation in large dimensions*, Journal of Computational Physics **354** (2018), 242–268.

[4] Martin V Day and Thomas A Darden, *Some regularity results on the Ventcel-Freidlin quasi-potential function*, Applied Mathematics and Optimization **13** (1985), no. 1, 259–282.

[5] Mathieu Desroches, John Guckenheimer, Bernd Krauskopf, Christian Kuehn, Hinke M Osinga, and Martin Wechselberger, *Mixed-mode oscillations with multiple time scales*, SIAM Review **54** (2012), no. 2, 211–288.

[6] Guo-Kang Er, *Methodology for the solutions of some reduced Fokker-Planck equations in high dimensions*, Annalen der Physik **523** (2011), no. 3, 247–258.

[7] Guo-Kang Er and Vai Pan Iu, *State-space-split method for some generalized Fokker-Planck-Kolmogorov equations in high dimensions*, Physical Review E **85** (2012), no. 6, 067701.

[8] Mark Iosifovich Freidlin and Alexander D Wentzell, *Random perturbations*, Random Perturbations of Dynamical Systems, Springer, 1998, pp. 15–43.

[9] John Guckenheimer and Radu Haiduc, *Canards at folded nodes*, Moscow Mathematical Journal **5** (2005), no. 1, 91–103.

[10] Martin Hairer and Jonathan C Mattingly, *Ergodicity of the 2d Navier-Stokes equations with degenerate stochastic forcing*, Annals of Mathematics (2006), 993–1032.

[11] Wen Huang, Min Ji, Zhenxin Liu, and Yingfei Yi, *Steady states of Fokker-Planck equations: I. existence*, Journal of Dynamics and Differential Equations **27** (2015), no. 3-4, 721–742.

[12] Ioannis Karatzas and Steven Shreve, *Brownian motion and stochastic calculus*, vol. 113, Springer Science & Business Media, 2012.

[13] Rafail Khasminskii, *Stochastic stability of differential equations*, vol. 66, Springer Science & Business Media, 2011.

[14] Tony Lelièvre and Gabriel Stoltz, *Partial differential equations and stochastic methods in molecular dynamics*, Acta Numerica **25** (2016), 681–880.

[15] Yao Li, *A data-driven method for the steady state of randomly perturbed dynamics*, Communications in Mathematical Sciences, accepted (2019).

[16] Yao Li and Yingfei Yi, *Systematic measures of biological networks I: Invariant measures and entropy*, Communications on Pure and Applied Mathematics **69** (2016), no. 9, 1777–1811.

[17] Andrew J Majda, Ilya Timofeyev, and Eric Vanden Eijnden, *A mathematical framework for stochastic climate models*, Communications on Pure and Applied Mathematics: A Journal Issued by the Courant Institute of Mathematical Sciences **54** (2001), no. 8, 891–974.

[18] Jonathan C Mattingly, Andrew M Stuart, and Michael V Tretyakov, *Convergence of numerical time-averaging and stationary measures via Poisson equations*, SIAM Journal on Numerical Analysis **48** (2010), no. 2, 552–577.

[19] Sean P Meyn and Richard L Tweedie, *Markov chains and stochastic stability*, Springer Science & Business Media, 2012.

[20] Bernt Øksendal, *Stochastic differential equations*, Stochastic differential equations, Springer, 2003, pp. 65–84.

[21] Hannes Risken, *Fokker-Planck equation*, The Fokker-Planck Equation, Springer, 1996, pp. 63–95.

[22] Yifei Sun and Mrinal Kumar, *A numerical solver for high dimensional transient Fokker-Planck equation in modeling polymeric fluids*, Journal of Computational Physics **289** (2015), 149–168.

[23] Utz von Wagner and Walter V Wedig, *On the calculation of stationary solutions of multi-dimensional Fokker-Planck equations by orthogonal functions*, Nonlinear Dynamics **21** (2000), no. 3, 289–306.

[24] EC Zeeman, *Stability of dynamical systems*, Nonlinearity **1** (1988), no. 1, 115.
