RICE UNIVERSITY

Solution of the Fokker-Planck Equation by Sequentially Optimized Meshfree Approximation

by

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ABSTRACT

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This thesis presents a technique to solve the Fokker-Planck equation by application of the Sequentially Optimized Meshfree Approximation (SOMA) method. It is well known that numerical solution of the Fokker-Planck equation is made difficult by the challenges of positivity enforcement, infinite domain, and high dimensionality. Through the use of optimization, radial basis functions, and its mesh-free architecture, respectively, the SOMA method attempts to address these challenges and sidestep the exponential growth of dimensionality, which hinders traditional numerical methods. Results are presented for one, two, and four-dimensional Fokker-Planck equations. This work will show that SOMA allows for enforcement of a positivity condition that removes the need for log-transforms, produces a solution domain that does not require artificial boundary condition enforcement, and provides the capability of solving higher dimensional forms of the Fokker-Planck equation.
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Nomenclature

Latin Characters

1 − $D$  one dimensional

2 − $D$  two dimensional

4 − $D$  four dimensional

c  basis function linear coefficient

$D$  diffusion coefficient

$f$  forcing function

$H[.]$  equation operator

$H^\alpha(\mathbb{R}^N)$  Sobolev space

$i, j$  indices

$k$  oscillator parameter

$K$  collocation points

$n$  number of basis functions

$n_p$  number of evaluation points

$N$  number of dimensions

$p$  probability density function
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<td>$p_A$</td>
<td>approximation of $p$</td>
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<td>$p_o$</td>
<td>initial condition</td>
</tr>
<tr>
<td>$R$</td>
<td>equation residual</td>
</tr>
<tr>
<td>$\mathbb{R}$</td>
<td>set of real numbers</td>
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<td>$t$</td>
<td>temporal variable</td>
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<td>$w$</td>
<td>constrained basis width parameter</td>
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<td>$x_N$</td>
<td>N-independent variables</td>
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### Greek Symbols

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<tr>
<td>$\beta$</td>
<td>basis width parameter</td>
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<td>$\gamma$</td>
<td>drift coefficient</td>
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<td>$\delta$</td>
<td>Dirac delta function</td>
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<tr>
<td>$\varepsilon$</td>
<td>merit function</td>
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<tr>
<td>$\zeta$</td>
<td>oscillator parameter</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>positivity enforcement value</td>
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<tr>
<td>$\xi_c$</td>
<td>basis center parameter</td>
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<td>$\sigma$</td>
<td>standard deviation</td>
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<tr>
<td>$\phi$</td>
<td>basis function</td>
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<td>$\omega$</td>
<td>oscillator frequency</td>
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**Acronyms**

<table>
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<th>Acronym</th>
<th>Description</th>
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<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>FPE</td>
<td>Fokker-Planck Equation</td>
</tr>
<tr>
<td>GRBF</td>
<td>Gaussian Radial Basis Function</td>
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<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>PDF</td>
<td>Probability Density Function</td>
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<tr>
<td>RMS</td>
<td>Root Mean Square</td>
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<td>SOMA</td>
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Chapter 1

Introduction

This thesis studies various forms of the Fokker-Planck Equation (FPE), an equation of motion for variables subject to stochastic excitation. Although it is only a second-order linear parabolic differential equation, the FPE presents unique difficulties of solution. The probability density is subjected to constraints of positivity and of normalization over an infinite domain. In addition, for many engineering applications, the number of problem dimensions can become quite large [1]. Unfortunately, the solution of the FPE for high dimensional systems has been limited by the architecture of traditional mesh-based numerical methods. This is commonly referred to in the literature as the “curse of dimensionality”, the phenomenon of increases in problem dimension leading to exponential increases in the computational resources required by traditional methods.

This thesis proposes a technique to solve the FPE by the application of the Sequentially Optimized Meshfree Approximation (SOMA) method, a nonlinear partial differential equation solver which does not use matrices, meshes, or volumes to store connectivity information. With SOMA, the strong form of partial differential equations are directly solved through the optimized addition of global basis functions. Because of this novel approach, the SOMA method promises to sidestep the exponential growth of dimensionality which hinders other numerical methods and provide a technique capable of solving the FPE for high dimensional systems. This capability is expected to advance the work being done on current aerodynamic optimization
problems described by stochastic models, such as those under geometric uncertainty [2].

1.1 Outline

First, the background of the FPE is given, and the challenges involved in its solution are discussed. Next, the Sequentially Optimized Meshfree Approximation method is presented. The overall architecture of the method is introduced, as well as the reasoning behind the selection of parameters which affect the performance of the method. Several numerical test cases are then presented: To benchmark the validity of the method, a solution is presented for the one dimensional FPE known as the Ornstein-Uhlenbeck process [3, 4, 5]. Selection of appropriate problem parameters is discussed, and convergence plots of the equation residual as well as the root mean square (RMS) error are presented. The method is then applied to a two dimensional FPE which has been well documented in the literature. Here, the advantages of SOMA’s ability to allow solutions with infinite domains are presented. The last numerical example is a four dimensional system which has been an active problem of interest in the solution of high dimensional Fokker-Planck equations. The effect of problem dimension on SOMA is discussed. Finally, future work to improve the Sequentially Optimized Meshfree Approximation method and its application to high dimensional Fokker-Planck equations is considered.
Chapter 2

The Fokker-Planck Equation

2.1 Formulation

Generally speaking, the motion of a single particle at the macroscopic level can be easily determined by classical physics. However, at the microscopic level, the vast number of particles and the number of collisions between them makes it impossible to determine the exact motion of an individual particle. In order to describe this motion, the sum of the microscopic collisions are treated macroscopically as a stochastic excitation, and the motion of the particle is described as a probability density. The FPE is an equation of motion for such variables subject to stochastic excitation.

By classification, the FPE is a second-order parabolic partial differential equation.*

The FPE describing a Markov process, generalized for $N$ dimensions, is:

$$
\frac{\partial p(\{x\}, t)}{\partial t} = \left[ -\sum_{i=1}^{N} \frac{\partial}{\partial x_i} D_i^{(1)}(\{x\}) + \sum_{i,j=1}^{N} \frac{\partial^2}{\partial x_i x_j} D_{ij}^{(2)}(\{x\}) \right] p(\{x\}, t) \quad (2.1)
$$

where $p(\{x\}, t)$ is the probability density function and $\{x\}$ is the vector of $N$ macroscopic variables (the sum of microscopic collisions). It should be noted that this equation could be generalized further, by including higher order derivatives to obtain

*It should be noted that there are two distinct formulations of the FPE; the Ito formulation, and the Stratonovich formulation. The Ito formulation requires the use of Ito integrals, and stochastic calculus. Consequently, the Ito formulation is more popular with mathematicians while the Stratonovich formulation is generally used by engineers. In this thesis, the Stratonovich formulation will be used.
the Kraymers-Moyal expansion, and also by including a temporal term to capture earlier time distributions and thus describe a non-Markovian process [4].

Structurally, the FPE consists of a second order derivative combined with a first order derivative; for a macroscopic equation of motion this combination is easily recognizable as acceleration and velocity. However, because of the stochastic excitation of the FPE and the fact that the particle of interest cannot usually be directly observed, it is more useful to represent those terms here as diffusion and drift, respectively.

2.2 Initial Conditions

The initial conditions that the FPE is subject to do not need to be precisely defined; because the system is subjected to stochastic excitation, it is impossible to define the system inputs with certainty. Instead, solutions are obtained for certain classes of excitation [4]. The most common stochastic excitation for which analytical solutions are available is Gaussian white noise, which is represented by the Dirac delta function.

$$\lim_{t \to 0} p(x) = \delta(x - x_0) \quad (2.2)$$

For the purposes of numerical modeling this initial condition is relaxed, and the delta function is approximated by a zero-mean Gaussian function [6]. Other representations, such as a binormal probability density function, are also commonly used [7].

It is important to note that if a stationary solution to a FPE exists, the choice of initial condition is trivial. It has been shown that any initial distribution will decay to the stationary solution, assuming some restrictions on the coefficients [4]. For these steady-state problems, the freedom to choose initial conditions allows for great flexibility in creating the numerical model.
2.3 Boundary Conditions

For the FPE there are four main types of boundary conditions. These are: (1) a reflecting wall condition, (2) an absorbing wall condition, (3) natural boundary conditions, and (4) periodic boundary conditions. Natural boundary conditions require that the probability density function (PDF), goes to zero for $x \pm \infty$; this is equivalent to a reflecting wall condition set at infinity. It is noted that stationary solutions only exist for systems with reflecting wall boundary conditions, including the special case of natural boundary conditions, and for systems with periodic boundary conditions [4]. The natural boundary conditions allow the range of the random variable to be infinite, and are appropriate for a wide variety of problems such as oscillator systems. Therefore, due to the existence of steady-state solutions and broad applicability, physical systems which require natural boundary conditions are the focus of the numerical modeling in this thesis.

One of the particular challenges encountered by researchers modeling the FPE is the task of enforcing the natural boundary conditions, which are defined over an infinite domain, on a finite numerical domain. One widely used method is to set Dirichlet conditions on a domain heuristically chosen to be large enough to capture the entire probability mass [8]. Penalty methods to enforce a boundary condition of either zero or an arbitrary small value have also been successfully used [9]. Although traditional Finite Difference and Finite Element formulations require the use of these methods, it will be shown in this work that the SOMA method, due to its global and mesh-free nature, does not require any boundary condition enforcement.
2.4 Normalization Condition

Due to the nature of probability density functions, which the FPE describes, additional constraints exist on the solution beyond the usual initial and boundary conditions. One of these is a normalization constraint, requiring that the volume of the probability density space equal one [4].

\[
\int_{-\infty}^{+\infty} p(x, t) dx = 1
\]  

(2.3)

This can be accomplished in multiple ways. The most common technique is to integrate the solution as a post processing step, then scale the magnitude of the solution to the correct value. A second method is to treat the FPE as an integro-differential equation, and thus obtain a solution which satisfies both the equation and the integral constraint at once. Both methods have been used in this thesis, and the results will be discussed in later sections.

2.5 Positivity Condition

Another constraint inherent to the solution of probability density functions is positivity [4, 10]. The justification of this constraint is captured in the physical meaning of the solution space; i.e. there can never be a negative probability that a particle has a certain position or velocity. A negative probability density value would be physically meaningless. Therefore the PDF is constrained between a probability of zero, or no possibility of occurrence, to a probability of one, which represents certainty of
occurrence.

\[ p(\{x\}, t) > 0 \]
\[ \{x\} \in \mathbb{R}^N, \forall t \]  \hspace{1cm} (2.4)

In summary, the normalization condition restricts the values of the density function from forming a sum which could represent a probability “greater” than certainty; likewise the positivity condition restricts the values of the density function from values which would represent a probability “less” than possible. Together, the normalization condition and the positivity condition prevent the equation from producing a physically meaningless solution.

This author has found that very few methods have been presented in the literature for enforcing positivity. Some researchers have reported using a log transform of the probability density function; however, this approach turns every problem into a nonlinear one, which is not desirable [11, 9]. In this thesis, a novel method of positivity enforcement will be reported. In addition, it will be shown that satisfying the integro-differential form of the FPE successfully implies positivity without direct enforcement.
Chapter 3

Sequentially Optimized Meshfree Approximation

3.1 Background

The Sequentially Optimized Meshfree Approximation (SOMA) method is a numerical method which is capable of solving nonlinear partial differential equations without storing connectivity data in matrices, meshes, or volumes. SOMA has already been proven as a successful Computational Fluid Dynamics solver, able to solve flows that are unsteady, compressible, and viscous [12]. Here, because of its mesh-free nature, use of infinitely continuous basis functions, and its optimization routine, SOMA is expected to avoid the problems associated with solving the FPE of dimensionality, finite boundary enforcement, and positivity, respectively. The architecture of the method will now be presented.

3.2 Form of the Approximation

In essence, SOMA is an optimal series expansion. The approximation to an $N$-dimensional function is built by the sequential addition of basis functions. If continuous basis functions are used to build the approximation, and analytical derivatives are used to build the equation operator, the result is a continuous, analytical approximation of the form:

$$p(x) \approx p_{A,n}(x) = p_o(x) + \sum_{i=1}^{n} c_i \phi_i(x, \xi_{c,i}, \beta_i)$$ (3.1)
Where \( p(x) \) is the exact solution, \( p_{A,n}(x) \) is the approximation built by \( n \) basis functions, \( \phi_i \) represents the \( ith \) basis function, and \( p_o(x) \) represents a function satisfying the initial conditions of the problem. The \( N \)-dimensional independent variables are represented by \( x \), and \( c, \xi_c, \beta \) represent respectively the linear coefficient, center location, and width of the basis function.

By storing the previous approximation \( p_{A,n-1}(x) \), the current approximation at the \( n \)th basis function can be written as:

\[
p_{A,n}(x) = c_n \phi_n(x, \xi_{c,n}, \beta_n) + p_{A,n-1}(x)
\]

\[
\text{(3.2)}
\]

### 3.3 Residual and Merit Function

SOMA is driven by selecting basis functions that minimize the residual of the approximation. The form of the residual for an \( n \)-basis approximation is given by:

\[
R_n(x) = H[p_{A,n}(x)] - f
\]

\[
\text{(3.3)}
\]

Where \( H[\cdot] \) is the equation operator and \( f \) is a forcing function. The residual \( R_n \) of the approximation is an analytical \( N \)-dimensional surface; therefore, a merit function is used to represent the residual by a scalar value that the optimization routine can minimize. The form of the merit function is:

\[
\varepsilon_n = \langle R_n, R_n \rangle
\]

\[
\text{(3.4)}
\]

where \( \langle \cdot, \cdot \rangle \) can be the integral inner product (i.e., method of weighted residuals), the sum root of the squares (i.e., collocation method), or another formulation.
collocation method is used in this work:

\[
\varepsilon_n = \sum_{j=1}^{n_p} R_n^2(x_j)
\]  

(3.5)

where \( n_p \) is the number of evaluation points. It is important to note that while the SOMA approximation is only expected to satisfy the equation residual at the evaluation points, the underlying approximation is analytical and continuous, meaning that evaluation points can be added, removed, or relocated at any time during the simulation.

### 3.4 Basis Function

![Example of a Gaussian Radial Basis Function](image)

Figure 3.1 : Example of a Gaussian Radial Basis Function

The basis function used in this work is the Gaussian Radial Basis Function, shown in Figure 3.1. This function was chosen because it can be completely defined with only three parameters, the linear coefficient \( c \), the \( N \)-dimensional center locations \( \xi_c \), and the width coefficient \( \beta \).
\[ c_i \phi_i = c_i \exp \left\{ -\beta_i^2 \| x_i - \xi_{c,i} \|^2 \right\} \]  \hspace{1cm} (3.6)

By defining:

\[ w = \exp \left\{ -\beta_i^2 \right\} \]  \hspace{1cm} (3.7)

Equation 3.6 can be rewritten as:

\[ c_i \phi_i = c_i w \left\{ \| x_i - \xi_{c,i} \|^2 \right\} \]  \hspace{1cm} (3.8)

Which has the advantage that the full range of \( w \) required to produce a GRBF is bounded between 0 → 1. Both Equation 3.6 and Equation 3.8 have been used in this work, based on convenience of their implementation in the optimization routines. In this thesis, the use of the term “width parameter” will be taken to mean either \( w \) or \( \beta \), as their use depends only on the form of the underlying basis function.

In addition, for linear equations, the height coefficient can be linearly separated from the nonlinear optimization and analytically calculated as:

\[ c_i = -\frac{\langle H [\phi_i], R_{n-1} \rangle}{\langle H [\phi_i], H [\phi_i] \rangle} \]  \hspace{1cm} (3.9)

The full derivation for this equation is given by Wilkinson [12].

For nonlinear problems, then, the Gaussian Radial Basis Function requires \( N + 2 \) parameters (\( N \) dimension centers, width, and \( c \)). For linear problems \( N+1 \) parameters are sufficient. Because the majority of SOMA’s computational resources are spent selecting basis parameters, this reduction in optimization problem size for the linear case is significant.
3.5 Derivatives

The derivatives used by SOMA in the equation operator $H[\cdot]$ have a significant impact on the accuracy and performance of the overall method.

For the special case of square domains and Dirichlet Boundary Conditions, analytical derivatives can be used along with appropriate boundary enforcer equations to set the boundary conditions. Analytical derivatives are desirable because they are extremely fast and accurate to machine precision ($\approx 10^{-16}$).

For Neumann conditions or irregular domains, either numerical or symbolic derivatives must be used. Symbolic derivatives, implemented here by MATLAB’s Symbolic Math Toolbox, were found to be accurate to machine precision. Qualitatively, they were slower than analytical or numerical derivatives to execute. Most importantly, however, the positivity enforcement employed by the optimization routine was unable to work with the symbolic calculations.

Several numerical derivative techniques were tested; qualitatively, these were found to be faster than the symbolic derivatives, although not accurate to machine precision, and able to support the positivity enforcement.

However, due to the use of radial basis functions, the problem in this thesis represents a special case of no boundary condition enforcement. Therefore analytical derivatives with no associated boundary enforcer equations were successfully utilized in this thesis. These represent the fastest, most accurate technique to build the function operator, and result in an approximation that is also analytical and continuous.
3.6 Error Convergence for Stationary Solutions

Meade and Zeldin [13] derived the limiting error estimate for the SOMA scheme given in Equation 3.10 for bell-shaped basis functions based on the L2 norm and the number of bases, $n$. For any function $p \in H^\alpha(\mathbb{R}^N)$, we can write,

$$\|p - p_{a,n}\|_2^2 \leq Cn^{-\alpha/N} \ln(n)$$

(3.10)

where $C$ is a constant that in practice depends only on the size of the approximation domain. The class of solutions which can be approximated by bell-shaped functions through SOMA, of which the Gaussian RBF is a member, is significantly larger and includes all square integrable functions. In addition, the bell-shaped basis approximation is applicable for a large class of bases, such as the piece wise linear basis, that are not restricted to infinitely smooth function.

For the highest derivative of the Fokker-Plank equation we can set $\alpha = N/2 + 1$. So the limiting rate of convergence of the approximation by bell-shaped functions is, apart from the slowing increasing factor $\ln(n)$, equal to $1/2 + 1/N$. This indicates that the SOMA algorithm will continue to converge to the exact solution at a rate no less than $1/2$ even as $N \to \infty$. Consequently, SOMA side-steps the curse of dimensionality. Of course, like all numerical algorithms, the problem of approximating a solution in an optimal manner becomes numerically unstable as $n \to \infty$. 

Chapter 4

Ornstein-Uhlenbeck Process

4.1 Formulation

The Ornstein-Uhlenbeck process models the Brownian motion of a free particle, and can be described by a FPE with constant diffusion coefficient and a linear drift coefficient. It is one of the simplest forms of the FPE, and has been well studied in the literature [3, 4, 5]. Because it is a Gaussian, Markov process, whose exact solution is readily available, it is an appealing and commonly chosen validation case for numerical solution techniques of stochastic differential equations.

The form of the governing equation for the Ornstein-Uhlenbeck process is:

\[
\frac{\partial p(x,t)}{\partial t} = \gamma \frac{\partial}{\partial x} [(x)p(x,t)] + D \frac{\partial^2}{\partial x^2} p(x,t)
\]  

(4.1)

where \( \gamma \) and \( D \) are the drift coefficient and the diffusion coefficient, respectively.

As expected for Fokker-Planck systems exhibiting an exact steady-state solution, the required initial condition is a family of Gaussian white noise excitations represented by the Dirac delta function. Although the Dirac delta function is a deterministic initial condition for the system, because it is not continuous it is not well suited to numerical implementation. The condition is therefore relaxed to a Gaussian distribution, which represents a stochastic initial condition.

As discussed in Section 2.2, the exact initial condition does not affect the sta-
tionary solution. The initial conditions are able to remain “uncertain”, while still leading to an appropriate stationary solution of the stochastic system. Here, the initial condition has been chosen to be:

$$p(x, 0) = \frac{1}{\sqrt{2\pi}} e^{-x^2} \quad (4.2)$$

The exact analytical solution at steady-state is given by

$$p(x, t \to \infty) = \sqrt{\frac{\gamma}{\pi \sigma^2}} e^{-\frac{\gamma(x-\mu)^2}{\sigma^2}} \quad (4.3)$$

where $\sigma = \sqrt{2D}$.

### 4.2 SOMA implementation

The domain of this problem was heuristically chosen to be $(-4, 4)$ to adequately capture the probability mass. For convenience, evaluation points were regularly placed throughout the domain with a discretization of 0.01.

The Genetic Algorithm from MATLAB’s Global Optimization Toolbox was used to select the center and width values of the radial basis function. The settings of the Genetic Algorithm specified the use of 1000 genes over 200 generations; these settings were chosen to provide fast convergence of the simulation.

The linear coefficient of the radial basis function was determined analytically, through the relationship given in Section 3.4. A plot of the linear coefficient versus basis function is shown in Figure 4.1. The decreasing trend of the height coefficient indicates that the simulation is progressing towards the optimal solution.

Positivity was enforced through the manipulation of the merit function evaluated by the genetic algorithm. By adding a conditional statement, the merit function from
Equation 3.5 becomes:

$$\varepsilon_n = \sum_{i=1}^{n_p} R_n^2(x_i), \quad p(x_1, x_2) > 0 \; \forall x_1, x_2$$  

(4.4)

$$\varepsilon_n = \kappa, \quad p(x_1, x_2) < 0 \; \forall x_1, x_2$$

Where $\kappa$ is a heuristically chosen large value. Because this condition on $\varepsilon_n$ occurs within the optimization routine, positivity is enforced with a negligible loss of efficiency.

Normalization was performed using trapezoidal integration. In order to show a history of the approximation error, this normalization was carried out after the addition of every basis function. Analytical derivatives of the initial condition and
basis function were used to determine the residual value of the equation for the given approximation. To validate the code, the true solution was input as an initial condition, and as expected the residual value was on the order of $10^{-16}$, or machine precision.

4.3 Results

The application of the SOMA method to the Ornstein-Uhlenbeck process produced numerical results that show accurate modeling of the probability density function. The approximation closely captured the analytical shape of the probability density function, as shown in Figure 4.2.

![Figure 4.2: One Dimensional FPE Normalized Approximation](image)

The square of the equation residual after 20 basis functions, shown in Figure 4.3,
is near machine precision.

In Figure 4.4, the RMS error between the approximation and the analytical solution shows a reduction of error to a value of $7.501 \times 10^{-4}$ after 20 basis functions.

The value of the merit function, $\varepsilon$, the parameter which drives the SOMA method, showed that the log scale convergence was better than linear, as presented in Figure 4.5.

In the literature, the moments which define the shape of a probability distribution are frequently used as a metric for accuracy, in particular the second central moment, or variance. The variance is a measure of how the probability distribution “spreads”, or varies, about the mean (the first raw moment). Figure 4.6 displays the magnitude of the difference between the variance of the true solution and the variance of the
Figure 4.4: RMS Error of Approximation to Analytical Solution

approximation. As the plot shows, the results agree well with the true solution.
Figure 4.5: Norm of Equation Residual ($\epsilon$) vs. Number of Basis Functions

Figure 4.6: Difference of Approximation Variance and True Variance with Increasing Number of Basis Functions
Chapter 5

Two Dimensional Linear System

5.1 Formulation

The bivariate PDF describing the velocity and position of a single degree-of-freedom linear oscillator is modeled by a two-dimensional FPE that has been well documented in the literature [7, 14].

The governing equation for this system is:

\[
\frac{\partial p(x_1, x_2, t)}{\partial t} = 2\zeta p - x_2 \frac{\partial p}{\partial x_1} + (2\zeta \omega x_2 + \omega^2 x_1) \frac{\partial p}{\partial x_2} + D \frac{\partial^2 p}{\partial x_2^2}
\] (5.1)

where the oscillator parameters commonly used in the literature are given as \( \zeta = 0.05 \) and \( \omega = 1 \).

The form of the initial condition used is given by:

\[
p(x_1, x_2, 0) = \frac{1}{\sqrt{2\pi \sigma}} e^{-\frac{1}{2\sigma}((x_1-\mu)^2+(x_2-\mu)^2)}
\] (5.2)

where the value of \( \sigma \) is chosen to be \( \frac{1}{3} \) and \( \mu \) is selected to be 1. These values were chosen heuristically, both to resemble those used in the literature and to fall within the smallest domain presented in these results; as discussed in Section 2.2, the choice of initial condition for a stationary solution is trivial.
5.2 Capabilities of the Infinite Domain

Evaluation points were placed at a discretization of 0.1 over the numerical domain. As discussed in Section 2.3, the use of Gaussian radial basis functions to build the approximation allows for great flexibility in the selection of the numerical domain. In order to demonstrate this, several numerical domains of different size were implemented.

In Figure 5.1, three separate simulations with square domains (-5,5), (-3,3), (-2.5,2.5) show that with no boundary condition enforcement, SOMA’s global approximation of the strong form governing equation is robust enough to allow for the use of very small domains. This is highly desirable for the reduction of problem size. In particular, the (-2.5,2.5) domain shows that SOMA is capable of obtaining the true solution, verified by the magnitude of the normalized approximation, even when the computational domain is smaller than the approximately non-constant regions of the probability density function.

5.3 SOMA implementation

The Genetic Optimization routine using 200 genes and 50 generations was again used to search for the radial basis function variables. As a two-dimensional problem, this required an $x_1$ center and an $x_2$ center in addition to the width parameter. The coefficient was again calculated analytically by the relationship given in Section 3.4.

Positivity was enforced in two different ways; by direct enforcement on the merit function, as presented in Equation 4.4 and by calculating the residual ($R$) of the integro-differential equation:
$$R = 2\zeta p - x_2 \frac{\partial p}{\partial x_1} + (2\zeta x_2 + x_1) \frac{\partial p}{\partial x_2} + D \frac{\partial^2 p}{\partial x^2} + \left| 1 - \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} p(x_1, x_2, t) dx_1 dx_2 \right|$$ (5.3)

Direct enforcement on the merit function was found to be faster, and is the method used in these results.

Normalization was accomplished as a post-processing step using double trapezoidal integration. It should be noted that when the residual modeled the integro-differential form of the equation, no normalization was required.

### 5.4 Results

The normalized approximation is shown in Figure 5.2. The figure shows that the value of $p(0, 0, \infty)$ is 0.1589. By comparison to the exact steady-state value of 0.15915 at the origin, the RMS error at this point is $1.768 \times 10^{-4}$. The square of the equation residual is displayed in Figure 5.3. As shown in Figure 5.4, the convergence of the simulation is initially better than linear.
Figure 5.1: Normalized Approximations Calculated with Domains
(a) (-5,5), (b) (-3,3), and (c) (-2.5,2.5)
Figure 5.2: Two Dimensional FPE Normalized Approximation

Figure 5.3: Distribution of Equation Residual Squared
Figure 5.4: Norm of Equation Residual ($\epsilon$) vs. Number of Basis Functions
Chapter 6

Four Dimensional Linear System

6.1 Formulation

The efficient solution of the four-dimensional Fokker Planck Equation is still a challenging problem. Here, a two degree-of-freedom system is presented which has been an active problem of interest in the solution of high dimension Fokker-Planck equations. The governing equation of the system is:

\[
\frac{\partial p}{\partial t} = D_1 \frac{\partial^2 p}{\partial x_1^2} + D_2 \frac{\partial^2 p}{\partial x_2^2} - x_2 \frac{\partial p}{\partial x_1} - x_4 \frac{\partial p}{\partial x_3} + (k_1 + k_2)x_1 \frac{\partial p}{\partial x_2} + c_1 x_2 \frac{\partial p}{\partial x_2} \\
- k_2 x_3 \frac{\partial p}{\partial x_2} - k_2 x_1 \frac{\partial p}{\partial x_4} + (k_2 + k_3)x_3 \frac{\partial p}{\partial x_4} + c_2 x_2 \frac{\partial p}{\partial x_4} + (c_1 + c_2)p
\]  

(6.1)

With initial conditions given by a multivariate Gaussian distribution of the form:

\[
p(x_1, x_2, x_3, x_4, 0) = \frac{1}{\sqrt{2\pi}} e^{-((x_1-\mu)^2+(x_2-\mu)^2+(x_3-\mu)^2+(x_4-\mu)^2)}
\]  

(6.2)

where \(\mu\) equals 0. The marginal initial condition is displayed in Figure 6.1.

6.2 SOMA implementation

In the literature, the numerical domain chosen for this system is typically \((-4, 4)\) along every dimension. However, the discretization used ranges from an ordered mesh of \(5^4\) to a mesh of \(41^4\) nodes [9, 15, 16]. For the results presented here, \(9^4\) SOMA evaluation points were placed regularly over the domain \((-4, 4)^4\). The optimization settings used
were 800 genes over 250 generations; these settings were chosen in order to adequately populate the initial generations for the increased number of optimization parameters (four center values and the width value).

6.3 Results

For a $9^4$ ordered grid of points, the full probability density function would require a display of $9^2$ two-dimensional plots; therefore only the marginal $x_1, x_2$ plot for $x_3 = 0, x_4 = 0$ is shown. Figure 6.2 shows the exact value for the marginal probability density function. Figure 6.3 shows the marginal probability density function approximation and Figure 6.4 shows the distribution of the corresponding residual squared error. The RMS error between the marginal approximation and true solution
is on the order of $10^{-3}$. This corresponds to an average nodal error is on the order of $10^{-5}$. While this error is only an indication of the method’s performance over one marginal slice of the multidimensional domain, Figure 6.5 shows the reduction of the norm of the equation residual, across the entire domain, with increasing number of basis functions. This is an extremely useful metric because the number of basis functions placed is independent of computational time; the plot effectively shows how well the optimization problem is being solved. It is clear from this plot that while the SOMA method extends to higher dimensions in a straightforward manner, the optimization problem that drives the technique becomes more difficult to solve because of the increasing number of optimization variables.

Figure 6.2 : Four Dimensional FPE Analytical Marginal PDF
Figure 6.3 : Four Dimensional FPE Approximation Marginal PDF

Figure 6.4 : Four Dimensional FPE Marginal Residual Squared
Figure 6.5: Norm of Equation Residual ($\epsilon$) vs. Number of Basis Functions
Chapter 7

Consideration of Transient Solutions and Nonlinear Systems

7.1 Two Dimensional Transient Solution

Figure 7.1: Transient Behavior of Two Dimensional FPE Approximation from $t = 0$ to 6.55 seconds

In order to display the efficacy of SOMA as a solution method for high dimensional Fokker-Planck equations, only stationary solutions have been considered in this thesis. However, study of the temporal solution can provide valuable insight into the behavior
of the FPE. For the two dimensional FPE studied in Chapter 5, the approximation of the temporal solution displayed at every time step from $t = 0 \rightarrow 6.55$ seconds is presented in Figure 7.1. For this simple demonstration, a backward-Euler time marching method with a time step of 0.05 seconds was found to be sufficient. Because the oscillator frequency, $\omega$, has a value of 1, the transient behavior of the PDF is expected to show a complete revolution every $2\pi$ seconds. As Figure 7.1 shows, this behavior is correctly captured by the SOMA method.

In Figure 7.2, the non-normalized PDF at $t = 38.5$ seconds is displayed, with the other time steps omitted for clarity. This PDF displays the expected symmetry about the origin characteristic of the stationary solution. The behavior of settling at an equilibrium distribution about a point is characteristic of Fokker-Planck equations, and is due to the combination of both a drift and diffusion term, as opposed to examples such as the Liouville equation, which does not have a diffusion term and whose solution continuously moves with time along a trajectory, or the Wiener process, which lacks a drift term and continuously spreads with relation to time [17].
7.2 Hardened Duffing Oscillator

7.2.1 Formulation

While this thesis has focused only on linear unimodal FPE systems, this section will present results for a nonlinear bimodal system, represented by a hardened Duffing Oscillator [16]. The governing equation for this system is given by:

\[
\frac{\partial p(x_1, x_2, t)}{\partial t} = 2\zeta \left( \left( x_2 \frac{\partial p}{\partial x_2} \right) + p \right) - x_1 \frac{\partial p}{\partial x_2} + \gamma \left( x_1^3 \right) \frac{\partial p}{\partial x_1} - x_2 \frac{\partial p}{\partial x_1} + (D_1 (x_1^2) + D_2) \frac{\partial^2 p}{\partial x^2}
\]  

(7.1)
where \( \zeta = 0.2, \gamma = 0.1, \) and \( D_2 = 0.4. \) For the case of no parametric excitation, presented here, \( D_1 = 0. \)

The initial condition is given by:

\[
p(x_1, x_2, 0) = e^{-\frac{1}{2}(x_1)^2 + (x_2)^2)}
\] (7.2)

The form of the exact stationary solution, for the case of no parametric excitation, is:

\[
p(x_1, x_2, t \to \infty) = e^{\frac{1}{2}(x_1)^2 - (x_2)^2 - \frac{1}{2} \gamma (x_1)^4)}
\] (7.3)

The contour plot of the initial condition is displayed in Figure 7.3.
7.2.2 SOMA Implementation

The numerical domain chosen here was (−10, 10) to match that used in the literature, although with the capability of SOMA discussed in Section 5.2 to solve over an infinite domain, a smaller domain could have been used to improve efficiency. The results shown here were calculated with an ordered grid of $33 \times 33$ evaluation points. Genetic algorithm settings of 200 genes and 100 generations were used.

7.2.3 Results

From comparison of Figure 7.4, which displays the approximate PDF, and Figure 7.5, which displays the exact PDF, it is clear that this simulation has difficulty capturing the “steepness” of the true solution. The location of the peaks of the bimodal distribution are correctly captured, but the width is not. As shown in Figure 7.6, the convergence of the simulation is initially worse than linear, then becomes linear after the addition approximately 100 basis functions. It is expected that these results could be improved through increasing the requirements of the genetic algorithm settings, or through the use of different basis functions to build the approximation.
Figure 7.4: Contour Plot of the Approximate PDF

Figure 7.5: Contour Plot of the Exact PDF
Figure 7.6 : Norm of Equation Residual Squared vs. Number of Basis Functions
Chapter 8

Future Work

8.1 Reduction of the Optimization Problem

Figure 8.1: Two Dimensional FPE Approximation using Collocation and Line-Search Optimization

The results presented in this thesis have shown the capabilities of SOMA as an optimal sequential approximation method. However, the computational cost associated with optimal performance may not be desirable when compared to the cost of a sub-optimal method. By creating a “sampling” matrix from the indices of an
$N$-dimensional array and a sample of widths that span the possible values of $w$ from $0 \rightarrow 1$, an $N$-dimensional basis center can be located without the need for optimizing $N + 1$ parameters. Because the centers will be restricted to the indices of the numerical grid, as collocation points ($K = 1, \ldots, n_p$), the method is not as optimal as allowing the basis centers to exist anywhere on the underlying infinite domain. However, the method will only require the optimization of one parameter, $w$, at the sub-optimal location. Therefore, regardless of the increase in dimension, SOMA’s optimization requirements will remain a simple line-search problem. For extremely high dimensional problems, it is expected that this suboptimal approach will be desirable due to the low computational cost of solving the line-search problem. Figures 8.1, 8.2, and 8.3 show the preliminary results of this technique as a proof of concept. Here, the
genetic algorithm was used to optimize $w$, treating the nodes of the numerical grid as collocation points.

Even though the method is sub-optimal, the convergence of Figure 8.3 is extremely good with just four basis functions; this can be attributed to the fact that the center of the initial condition distribution, given in Equation 5.2, and the center of the stationary probability density, shown in Figure 5.2, both happen to coincide with collocation points. Thus, if some of the behavior of the underlying model is already known, these results show that the use of collocation points can be tailored even further to improve the efficiency of the method.
8.2 Intelligent Tuning of Optimization Parameters

The performance of the optimization routine is directly related to the performance of the SOMA method. One area where the optimization routine could be improved is in the “tuning” values which the operator specifies for the simulation. These tuning values exist for two reasons: (1) in order to make the search space a hypercube, which is necessary for efficient operation of the genetic algorithm, and (2) in order to restrict the search space to only the space where the parameters can exist. However, the space where the parameters can exist changes with the approximation. By studying Figures 8.4 and 8.5, which represents the search parameters from the two-dimensional results given in Chapter 5, it is clear that there is a relationship between the progression of the approximation and the range of the search parameters. These relationships could be exploited in future work to improve the performance SOMA.

Figure 8.4 : Width Coefficient vs. Number of Basis Functions for 2-D FPE
Figure 8.5: Linear Coefficient vs. Number of Basis Functions for 2-D FPE
Chapter 9

Conclusions

It has been shown that Sequentially Optimized Meshfree Approximation can successfully overcome the three major challenges of solving the FPE. Due to the optimization routine at its core, the method allows for enforcement of a positivity condition that removes the need for log-transforms or penalty methods. Additionally, due to the use of global radial basis functions to build the approximation, the solution domain is infinite and no artificial boundary condition enforcement is required. These two constraints, which are frequently discussed in the literature as major challenges to the solution of the FPE, present no challenge for SOMA.

Finally, the method presented here can be directly extended to any dimension. Although it is expected that dimensions much higher than four could be solved immediately through implementation of this method in lower-level programming languages and through use of supercomputer resources, current work in progress promises to reduce the optimization requirements to a line-search problem, making it feasible to solve high dimension Fokker-Planck equations with desktop computing resources.
Bibliography


