2009 American Control Conference
Hyatt Regency Riverfront, St. Louis, MO, USA
June 10-12, 2009

Model Predictive Control of Nonlinear Stochastic PDEs: Application to a Sputtering Process

Yiming Lou, Gangshi Hu and Panagiotis D. Christofides

Abstract— **In this work, we develop a method for model predictive control of nonlinear stochastic partial differential equations (PDEs) to regulate the state variance, which physically represents the roughness of a surface in a thin film growth process, to a desired level. We initially formulate a nonlinear stochastic PDE into a system of infinite nonlinear stochastic ordinary differential equations (ODEs) by using Galerkin's method. A finite-dimensional approximation is then derived that captures the dominant mode contribution to the state variance. A model predictive control problem is formulated based on the finite-dimensional approximation so that the future state variance can be predicted in a computationally efficient way. The control action is computed by minimizing an objective function including penalty on the discrepancy between the predicted state variance and a reference trajectory, and a terminal penalty. An analysis of the closed-loop nonlinear infinite-dimensional system is performed to characterize the closed-loop performance enforced by the model predictive controller. The model predictive controller is initially applied to the stochastic Kuramoto-Sivashinsky equation (KSE), a fourth-order nonlinear stochastic PDE. Simulation results demonstrate that the proposed predictive controller can successfully drive the norm of the state variance of the stochastic KSE to a desired level in the presence of significant model parameter uncertainties. In addition, we consider the problem of surface roughness regulation in a one-dimensional ion-sputtering process. The predictive controller is applied to the kinetic Monte Carlo model of the sputtering process to successfully regulate the expected surface roughness to a desired level.**

I. Introduction

Nonlinear stochastic partial differential equations (PDEs) arise naturally in the modeling of the evolution of the surface height profile of ultra thin films in a variety of material preparation processes such as thin film growth [5], [10], [23], [24] and ion sputtering processes [6], [13]. Recently, it was demonstrated that covariance control methods can be applied to stochastic PDEs and result in successful control of microscopic thin film morphology and methods for feedback control of surface roughness based on linear [16], [17] and nonlinear [18] stochastic PDE process models were developed. These stochastic-PDE-based control methods constitute an alternative to control of thin film microstructure based on kinetic Monte-Carlo models [14], [15]. Furthermore, a systematic identification approach was developed for linear stochastic PDEs [16] and methods for construction of linear and nonlinear stochastic PDE models for thin film growth and ion-sputtering processes using first principles-based microscopic simulations were proposed [12], [20].

Model predictive control (MPC) is widely used in chemical process control due to its capability to handle input and state constraints, to tolerate model uncertainty and suppress external disturbances, and to force the closed-loop system to follow a target trajectory using optimal control action (see References [2], [11], [21], [22] for surveys of results and references in this area). In MPC, the control action is obtained by repeatedly solving an on-line finite horizon constrained open-loop optimal control problem. Recent efforts on predictive control of distributed parameter systems have focused on predictive control of deterministic parabolic PDEs including linear systems with distributed [9] and boundary [7] control and nonlinear systems with distributed control [8]. However, results on predictive control of stochastic distributed parameter systems, to the best of our knowledge, are not available.

In this work, a method for model predictive control of nonlinear stochastic PDEs is developed. The control objective is to regulate the state variance of the stochastic PDE to a desired level. A nonlinear stochastic PDE is first formulated into an infinite-dimensional nonlinear stochastic ODE system by using Galerkin's method. A finite-dimensional approximation is then constructed to capture the dominant mode contribution to the state variance. A model predictive control problem is formulated based on the finite-dimensional approximation.The control action is computed by minimizing an objective cost function, which includes both in-process and terminal penalties. An analysis of the closed-loop nonlinear infinite-dimensional system is performed to characterize the closed-loop performance enforced by the model predictive controller. Finally, numerical simulations are performed to the stochastic KSE model and the kinetic Monte Carlo model of an ion-sputtering process to demonstrate the effectiveness and the robustness of the proposed predictive controller.

II. Preliminaries

We consider nonlinear dissipative stochastic PDEs with distributed control of the following form:

$$\frac{\partial h}{\partial t} = \mathscr{A}h + \mathscr{F}(h) + \sum_{i=1}^{p} b_i(x)u_i(t) + \xi(x,t) \qquad (1)$$

Yiming Lou is with Hamilton Sundstraud United Technologies Corporation, 2771 North Garey Avenue, Pomona, CA 91767 USA; e-mail: ylou@ieee.org.

Gangshi Hu is with the Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, CA 90095 USA.

Panagiotis D. Christofides is with the Department of Chemical and Biomolecular Engineering and the Department of Electrical Engineering, University of California, Los Angeles, CA 90095 USA.

Panagiotis D. Christofides is the corresponding author: Tel: +1(310)794-1015; Fax: +1(310)206-4107; e-mail: pdc@seas.ucla.edu.

Financial support from NSF, CBET-0652131, is gratefully acknowledged by Gangshi Hu and Panagiotis D. Christofides.

978-1-4244-4524-0/09/$25.00 ©2009 AACC

subject to homogeneous boundary conditions and the initial condition $h(x,0) = h_0(x)$, where $x \in [-\pi, \pi]$ is the spatial coordinate, t is the time, $h(x,t)$ is the height of the surface at position x and time t, $\mathscr{A}$ is a dissipative spatial differential operator, $\mathscr{F}$ is a nonlinear function, $u_i(t)$ is the i^{th} manipulated input, p is the number of manipulated inputs and $b_i(x)$ is the i^{th} actuator distribution function (i.e., $b_i(x)$ determines how the control action computed by the i^{th} control actuator, $u_i(t)$, is distributed (e.g., point or distributed actuation) in the spatial interval $[-\pi, \pi]$). $\xi(x,t)$ is a Gaussian noise with zero mean and the following expression for its covariance:

$$\langle \xi(x,t)\xi(x',t')\rangle \quad = \quad \sigma^2 \delta(x-x')\delta(t-t') \tag{2}$$

where σ is a real number, $\delta(\cdot)$ is the Dirac delta function, and $\langle\cdot\rangle$ denotes the expected value.

The eigenvalue problem for $\mathscr{A}$ is defined as

$$\mathscr{A}\bar{\phi}_j \quad = \quad \lambda_j \bar{\phi}_j, \quad j = 1, 2, \cdots, \infty \tag{3}$$

where λ_j and $\bar{\phi}_j$ denote the jth eigenvalue and eigenfunction, respectively. To simplify our development and motivated by most practical applications, we consider stochastic PDEs for which $\mathscr{A}$ is a highly dissipative operator (i.e., a second-order or fourth-order linear self-adjoint operator) and has eigenvalues which are real numbers and eigenfunctions which are orthogonal to each other. The eigenspectrum of $\mathscr{A}$, $\sigma(\mathscr{A})$, is defined as the set of all eigenvalues of $\mathscr{A}$, i.e. $\sigma(\mathscr{A}) = \{\lambda_1, \lambda_2, \cdots\}$. Assumption 1 states that the eigenspectrum of $\mathscr{A}$ can be partitioned into a finite-dimensional part consisting of m slow eigenvalues and a stable infinite-dimensional complement containing the remaining fast eigenvalues, the separation between the slow and fast eigenvalues of $\mathscr{A}$ is large, and that the infinite sum of $\sum_{i=1}^{\infty} 1/|\lambda_i|$ converges to a finite positive number.

Assumption 1: The eigenvalues of $\mathscr{A}$ satisfy the following [4]:

1) $\lambda_1 \geq \lambda_2 \geq \ldots$.
2) $\sigma(\mathscr{A})$ can be partitioned as $\sigma(\mathscr{A}) = \sigma_1(\mathscr{A}) + \sigma_2(\mathscr{A})$, where $\sigma_1(\mathscr{A})$ consists of the first m (with m finite) eigenvalues, i.e. $\sigma_1(\mathscr{A}) = \{\lambda_1, \lambda_2, \cdots, \lambda_m\}$. $\lambda_{m+1} < 0$ and $\frac{|\lambda_1|}{|\lambda_{m+1}|} = O(\varepsilon)$ where $\varepsilon < 1$ is a small positive number.
3) There exists a positive number, $\gamma > 0$, such that for sufficient large n, $\sum_{i=n}^{\infty} \frac{1}{|\lambda_i|} < \gamma$.

Note that the eigenvalue problem of the stochastic PDE of Eq.1 is formulated in the same way as that of deterministic PDEs. The assumption of finite number of unstable eigenvalues and discrete eigenspectrum are always satisfied for parabolic PDE systems defined in finite spatial domains [3], while the assumption of existence of only a few dominant modes that capture the dominant dynamics of the stochastic parabolic PDE system and the convergence of the infinite sum $\sum_{i=n}^{\infty} 1/|\lambda_i|$ to a finite positive number are usually satisfied by the majority of materials processes (see the example of the sputtering process described by the stochastic Kuramoto-Sivashinsky equation in the Simulation section).

III. Nonlinear Model Predictive Controller Design

A. Model reduction

We apply Galerkin's method to the system of Eq.1 to derive an approximate finite-dimensional system. First, the solution of Eq.1 is expanded into an infinite series in terms of the eigenfunctions of the operator $\mathscr{A}$ of Eq.3 as follows:

$$h(x,t) = \sum_{n=1}^{\infty} \alpha_n(t)\bar{\phi}_n(x) \tag{4}$$

where $\alpha_n(t)$ are time-varying coefficients. Substituting the above expansion for the solution, $h(x,t)$, into Eq.1 and taking the inner product with the adjoint eigenfunctions, $\bar{\phi}_n^*(x)$, the following system of infinite nonlinear stochastic ODEs is obtained:

$$\frac{d\alpha_n}{dt} = \lambda_n \alpha_n + f_{n\alpha} + \sum_{i=1}^{p} b_{i\alpha_n} u_i(t) + \xi_\alpha^n(t), \quad n = 1, \ldots, \infty \tag{5}$$

where

$$b_{i\alpha_n} = \int_{-\pi}^{\pi} \bar{\phi}_n^*(x) b_i(x) dx, \quad \xi_\alpha^n(t) = \int_{-\pi}^{\pi} \xi(x,t)\bar{\phi}_n^*(x) dx \tag{6}$$

and

$$f_{n\alpha} = \int_{-\pi}^{\pi} \bar{\phi}_n^*(x) \mathscr{F}(h) dx \tag{7}$$

Note that the operator $\mathscr{A}$ is self-adjoint, therefore, the adjoint eigenfunction is equal to the corresponding eigenfunction, i.e., $\bar{\phi}_n^*(x) = \bar{\phi}_n(x)$.

Due to the orthogonality of the eigenfunctions of operator $\mathscr{A}$, the projections of the noise, $\xi_\alpha^n(t)$, are independent stochastically. As integrals of white noise, the covariances of $\xi_\alpha^n(t)$ can be computed by using the following result:

Result 1: If (1) $f(x)$ represents a general deterministic function, (2) $\eta(x)$ is a random variable with $\langle\eta(x)\rangle = 0$ and covariance $\langle\eta(x)\eta(x')\rangle = \sigma^2\delta(x-x')$, and (3) $\varepsilon = \int_a^b f(x)\eta(x)dx$, then ε is a real random number with $\langle\varepsilon\rangle = 0$ and covariance $\langle\varepsilon^2\rangle = \sigma^2 \int_a^b f^2(x)dx$ [1].

Owing to its infinite-dimensional nature, the system of Eq.5 cannot be directly used for the design of controllers that can be implemented in practice (i.e., the practical implementation of controllers which are designed on the basis of this system will require the computation of infinite sums which cannot be done by a computer). Instead, we will base the controller design on a finite-dimensional approximation of this system. Subsequently, we will show that the resulting controller will enforce the desired control objective in the closed-loop infinite-dimensional system. Specifically, we rewrite the system of Eq.5 as follows:

$$\begin{aligned} \frac{dx_s}{dt} &= \mathscr{A}_s x_s + \mathscr{F}_s(x_s, x_f) + \mathscr{B}_s u + \xi_s \\ \frac{dx_f}{dt} &= \mathscr{A}_f x_f + \mathscr{F}_f(x_s, x_f) + \mathscr{B}_f u + \xi_f \end{aligned} \tag{8}$$

where $x_s = [\alpha_1 \ \alpha_2 \ \cdots \ \alpha_m]^T$, $x_f = [\alpha_{m+1} \ \alpha_{m+2} \ \cdots]^T$, $\mathscr{A}_s = diag[\lambda_1 \ \lambda_2 \ \cdots \ \lambda_m]$, $\mathscr{A}_f = diag\ [\lambda_{m+1} \ \lambda_{m+2} \ \cdots]$, $\mathscr{F}_s(x_s,x_f) = [f_{1\alpha}(x_s,x_f) \quad f_{2\alpha}(x_s,x_f) \quad \cdots \quad f_{m\alpha}(x_s,x_f)]^T$, $\mathscr{F}_f(x_s,x_f) = [f_{m+1\alpha}(x_s,x_f) \ \ f_{m+2\alpha}(x_s,x_f) \ \cdots]^T$, $u = [u_1 \quad u_2 \quad \cdots \quad u_p]$, $\xi_s = [\xi_\alpha^1 \quad \cdots \quad \xi_\alpha^m]$, and $\xi_f = [\xi_\alpha^{m+1} \quad \xi_\alpha^{m+2} \quad \cdots]$.

The standard Galerkin's method is to approximate the solution $h(x,t)$ of the system of Eq.1 by $\tilde{x}_s(t)$, which is given by the following $m-$dimensional system:

$$\frac{d\tilde{x}_s}{dt} = \mathscr{A}_s\tilde{x}_s + \mathscr{F}_s(\tilde{x}_s,0) + \mathscr{B}_s u + \xi_s \tag{9}$$

where the tilde symbol in $\tilde{x}_s$ denotes that this state variable is associated with a finite-dimensional system.

B. Predictive controller design

In this section, we design a nonlinear model predictive controller based on the finite-dimensional stochastic ODE system of Eq.9 to control the norm of the state variance of the nonlinear stochastic infinite-dimensional system of Eq.1 to a desired level. Let $X = [x_s^T \ x_f^T]^T$. The variances of x_s, x_f and X are defined as:

$$\begin{array}{rcl} var(x_s(t)) & = & \left[\ \langle\alpha_1(t)^2\rangle \quad \cdots \quad \langle\alpha_m(t)^2\rangle \ \right]^T \\ var(x_f(t)) & = & \left[\ \langle\alpha_{m+1}(t)^2\rangle \quad \langle\alpha_{m+2}(t)^2\rangle \quad \cdots \ \right]^T \\ var(X(t)) & = & \left[\ var(x_s(t))^T \quad var(x_f(t))^T \ \right]^T \end{array} \tag{10}$$

where $\langle\cdot\rangle$ denotes the expected value.

We provide a predictive control formulation that is on the basis of the finite-dimensional system of Eq.9 and computes the control action by minimizing an objective function including the distance between the predicted state variance and a reference trajectory and a terminal penalty.

Consider a vector of reference trajectories describing the desired trajectories for each element of the variance of x_s, $var(x_s^*(t)) = [\langle\alpha_1^*(t)^2\rangle \ \cdots \ \langle\alpha_m^*(t)^2\rangle]^T$. The control action, $u(t)$, can be obtained by solving, in a receding horizon fashion, the following optimization problem:

$$\begin{array}{c} \min\limits_u \int_t^{t+T_p} \left(Q\|var(\tilde{x}_s^u(\tau)) - var(x_s^*(\tau))\|^2 + R\|u(t)\|^2\right) d\tau \\ +Q_f\|var(\tilde{x}_s^u(t+T_p)) - var(x_s^*(t+T_p))\|^2 \\ s.t. \\ \dfrac{d\tilde{x}_s}{dt} \quad = \quad \mathscr{A}_s\tilde{x}_s + \mathscr{F}_s(\tilde{x}_s,0) + \mathscr{B}_s u + \xi_s \end{array} \tag{11}$$

where Q and Q_f are positive real numbers, T_p is the prediction horizon, and $\tilde{x}_s^u(\tau)$ is the solution of Eq.9 that is due to the control $u(\tau)$, with an initial condition $\tilde{x}_s(t)$ at a time t.

A challenge for the design of a predictive controller for a stochastic process is to predict the state variance, $var(x_s(t))$, in a computationally efficient way. Although a realization of the future evolution of state variance can be solved through numerical integrations of the stochastic process model, due to the stochastic nature of the process, numerical solutions from different simulation runs of the same stochastic process are not identical. The state variance should be computed by averaging the numerical solutions of the stochastic process from a large number of individual simulation runs. The prediction of state variance using brute force numerical integration of a nonlinear stochastic system is, therefore, extremely computationally expensive and is not appropriate for the design of predictive controllers to be implemented in real-time.

As an alternative, an analytical solution of the state variance based on the process model, if available, provides a feasible way for MPC design. For linear stochastic PDEs, the analytical solution of the state variance is readily available, which results in efficient design of a model predictive controller for surface variance regulation [20]. However, analytical solutions of the state variance for nonlinear stochastic PDEs are, in general, not available. To this end, we focus on the construction of a nonlinear feedback controller that can induce a linear structure in the closed-loop finite-dimensional stochastic system of Eq.9. Therefore, the analytical solution of the state variance under the proposed controller structure can be obtained. Consequently, the control action is computed by solving an optimization problem in a receding horizon fashion and computationally efficient way.

Specifically, the control law takes the following form:

$$u(t) \quad = \quad \mathscr{B}_s^{-1}\left\{(\mathscr{A}_{cs}(t) - \mathscr{A}_s)\tilde{x}_s(t) - \mathscr{F}_s(\tilde{x}_s(t),0)\right\} \tag{12}$$

where $\mathscr{A}_{cs}(t) = diag[\lambda_{c1}(t) \ \cdots \ \lambda_{cm}(t)]$, $\lambda_{ci}(t)$ $(1 \le i \le m)$ are time-varying, desired poles of the closed-loop finite-dimensional system. Note that in the proposed controller structure of Eq.12, the desired poles are not fixed values but will be computed in real-time by solving an on-line optimization problem in a receding horizon fashion. This is a fundamental difference from the nonlinear feedback controller proposed in our previous work [18].

Replacing the u of Eq.9 by Eq.12, we have the following closed-loop system:

$$\frac{d\tilde{x}_s(t)}{dt} = \mathscr{A}_{cs}(t)\tilde{x}_s(t) + \xi_s \tag{13}$$

In this control problem formulation, the computation of the control action, $u(t)$, is equivalent to the computation of $\mathscr{A}_{cs}(t)$, or the values of $\lambda_{ci}(t)$ for $i = 1,2,\cdots,m$, by solving the following optimization problem:

$$\begin{array}{c} \min\limits_{\mathscr{A}_{cs}(t)} \int_t^{t+T_p} \left(Q\|var(\tilde{x}_s(\tau)) - var(x_s^*(\tau))\|^2\right) d\tau \\ +Q_f\|var(\tilde{x}_s(t+T_p)) - var(x_s^*(t+T_p))\|^2 \\ s.t. \\ \dfrac{d\tilde{x}_s}{dt} = \mathscr{A}_{cs}(t)\tilde{x}_s + \xi_s \\ \\ a_i < \lambda_{ci}(t) < b_i; \quad i = 1,2,\cdots,m. \end{array} \tag{14}$$

Note that in the optimization problem of Eq.14, $\mathscr{A}_{cs}(t)$ does not change during the optimization time interval $t < \tau < t + T_p$. The control action, u, is computed based on the solution of the constrained optimization problem of Eq.14 using Eq.12. Therefore, u is not explicitly included in the objective function. The system of Eq.13 is a linear stochastic system and the analytical solution of the state variance of

Eq.13 can be obtained as follows:

$$\tilde{x}_n(\tau) = e^{\lambda_{cn}(\tau-t)}\tilde{x}_n(t) + \int_t^{\tau} e^{\lambda_{cn}(t+T_p-\mu)}\xi_s^n(\mu)d\mu \quad ;n=1,2,\cdots,m. \tag{15}$$

The expected value (the first stochastic moment) and the variance (the second stochastic moment) of the state of Eq.13 can be computed as follows [16], [20]:

$$\begin{aligned} \langle \tilde{x}_n(\tau)\rangle &= e^{\lambda_{cn}(\tau-t)}\tilde{x}_n(t) \\ \langle \tilde{x}_n(\tau)^2\rangle &= \frac{e^{2\cdot\lambda_{cn}(\tau-t)}-1}{2\cdot\lambda_{cn}} + \langle \tilde{x}_n(t)\rangle^2 \quad ;n=1,2,\cdots,m. \end{aligned} \tag{16}$$

Eq.16 gives the analytical solution of $var(\tilde{x}_s(t))$ in the closed-loop finite-dimensional system of Eq.9. Using Eq.16, the optimization problem of Eq.14 can be subsequently formulated as a minimization of a nonlinear algebraic equation, which can be readily solved by using standard unconstrained or constrained multidimensional nonlinear minimization algorithms (for example, Nelder-Mead method or golden section search).

By applying the controller of Eqs.12 and 14 to the infinite-dimensional system of Eq.8, and using that $\varepsilon = \frac{|\lambda_1|}{|\lambda_{m+1}|}$, the closed-loop system takes the form:

$$\begin{aligned} \frac{dx_s}{dt} &= \mathscr{A}_{cs}x_s + (\mathscr{F}_s(x_s,x_f) - \mathscr{F}_s(x_s,0)) + \xi_s \\ \varepsilon\frac{dx_f}{dt} &= \mathscr{A}_{f\varepsilon}x_f + \varepsilon\mathscr{B}_f\mathscr{B}_s^{-1}(\mathscr{A}_{cs}-\mathscr{A}_s)\tilde{x}_s \\ &\quad +\varepsilon\mathscr{F}_f(x_s,x_f) - \varepsilon\mathscr{B}_f\mathscr{B}_s^{-1}\mathscr{F}_s(\tilde{x}_s,0) + \varepsilon\xi_f \end{aligned} \tag{17}$$

where λ_1 and λ_{m+1} are the first and the $(m+1)th$ eigenvalues of the linear operator in Eq.8, and $\mathscr{A}_{f\varepsilon} = diag[\lambda_{\varepsilon 1}\ \lambda_{\varepsilon 1}\ \lambda_{\varepsilon 2}\ \lambda_{\varepsilon 2}\ \cdots]$ is an infinite-dimensional matrix defined as $\mathscr{A}_{f\varepsilon} = \varepsilon\cdot\mathscr{A}_f$.

We now proceed to characterize the accuracy with which the variance of $X = [x_s^T\ x_f^T]^T$ is controlled in the closed-loop infinite-dimensional system. Theorem 1 provides estimates of the variances of x_s and x_f of the closed-loop system of Eq.17 and a characterization of the variance of X enforced by the controller of Eqs.12 and 14 in the closed-loop infinite dimensional system. The proof of Theorem 1 can be found in the journal version of this paper [19] and is omitted here due to space limitation.

Theorem 1: Consider the closed-loop stochastic infinite-dimensional system of Eq.17 and the definition of $\|var(x_s)\|^2$, $\|var(x_f)\|^2$, and $\|var(X)\|^2$ shown in Eq.10. Then, there exist $\mu^* > 0$ and $\varepsilon^* > 0$ such that if $\|x_{f0}\| + \|x_{s0}\| \le \mu^*$ and $\varepsilon \in (0,\varepsilon^*]$, $\|var(x_s(t_f))\|^2$, $\|var(x_f(t_f))\|^2$, and $\|var(x(t_f))\|^2$ satisfy:

$$\|var(x_f(t))\|^2 = O(\varepsilon) \tag{18}$$

$$\|var(x_s(t))\|^2 = \|var(x_s^*(t))\|^2 + O(\sqrt{\varepsilon}) \tag{19}$$

$$\|var(X(t))\|^2 = \|var(x_s^*(t))\|^2 + O(\sqrt{\varepsilon}) \tag{20}$$

where x_{f0} and x_{s0} are the initial conditions for x_f and x_s in Eq.17, respectively.

Remark 1: Referring to the closed-loop finite-dimensional system, we note that the predictive controller of Eq.11 needs to be carefully designed to ensure closed-loop stability. Specifically, let's consider the closed-loop stochastic finite-dimensional system of Eq.9. Its stability is determined by the term $\mathscr{A}_s\tilde{x}_s + \mathscr{F}_s(\tilde{x}_s,0) + \mathscr{B}_s u$ and is not affected by the noise term ξ_s. Therefore, the closed-loop stability of the stochastic finite-dimensional system under predictive control can be addressed in the context of predictive control of deterministic systems (see [2], [21], [22] for results on predictive control of finite-dimensional systems and [8], [9] for results on predictive control of infinite-dimensional systems). A stabilizing predictive controller can be designed by imposing suitable weight matrices (Q, R and Q_f) and using an appropriate prediction horizon.

IV. Simulation results

In this section, we present applications of the proposed model predictive controller to both the stochastic Kuramoto-Sivashinsky equation (KSE), a fourth order nonlinear stochastic PDE model, and the kinetic Monte Carlo model of a sputtering process. Since the physical interpretation of the state variance of a stochastic PDE is the expected roughness of the surface modeled by the stochastic PDE, we will use the expected surface roughness as the control objective in the simulation study. Simulation results demonstrate that the proposed model predictive controller is able to regulate the expected surface roughness of the process modeled by the stochastic KSE to a desired level with good robustness properties against model uncertainties. Furthermore, we demonstrate that the controller designed based on the stochastic KSE model of the process can regulate the surface roughness of the kinetic Monte Carlo model of the same process to a desired level.

A. Nonlinear predictive control of the stochastic Kuramoto-Sivashinsky equation

The stochastic KSE is a fourth-order nonlinear stochastic PDE that describes the evolution of the height fluctuation for surfaces in a variety of material preparation processes including surface erosion by ion sputtering, surface smoothing by energetic clusters and ZrO_2 thin film growth by reactive ion beam sputtering. We consider the following stochastic KSE with spatially distributed control:

$$\frac{\partial h}{\partial t} = -\nu\frac{\partial^2 h}{\partial x^2} - \kappa\frac{\partial^4 h}{\partial x^4} + \frac{\lambda}{2}\left(\frac{\partial h}{\partial x}\right)^2 + \sum_{i=1}^{p}\hat{b}_i(x)u_i(t) + \xi'(x,t) \tag{21}$$

where u_i is the i^{th} manipulated input, p is the number of manipulated inputs, $\hat{b}_i$ is the i^{th} actuator distribution function (i.e., $\hat{b}_i$ determines how the control action computed by the i^{th} control actuator, u_i, is distributed (e.g., point or distributed actuation) in the spatial interval $[-\pi,\pi]$), $\nu = 1.975\times10^{-4}$, $\kappa = 1.58\times10^{-4}$, $\lambda = 1.975\times10^{-4}$, $x\in[-\pi,\pi]$ is the spatial coordinate, t is the time, $h(x,t)$ is the height of the surface

at position x and time t and $\xi'(x,t)$ is a Gaussian noise with zero mean and unit covariance:

$$\langle \xi'(x,t)\xi'(x',t')\rangle \quad = \quad \delta(x-x')\delta(t-t') \tag{22}$$

A $200th$ order stochastic ODE of Eq.21 obtained via Galerkin's method is used to simulate the process (the use of higher-order approximations led to identical numerical results, thereby implying that the following simulation runs are independent of the discretization). The δ function involved in the covariances of ξ_α^n and ξ_β^n is approximated by $\frac{1}{\Delta t}$, where Δt is the integration time step.

1) Eigenvalue problem: To study the dynamics of Eq.21, we initially consider the eigenvalue problem of the linear operator of Eq.21, which takes the form:

$$A\bar{\phi}_n(x) = -\nu\frac{d^2\bar{\phi}_n(x)}{dx^2} - \kappa\frac{d^4\bar{\phi}_n(x)}{dx^4} = \lambda_n\bar{\phi}_n(x)$$

$$\frac{d^j\bar{\phi}_n}{dx^j}(-\pi) = \frac{d^j\bar{\phi}_n}{dx^j}(+\pi); \quad j=0,\cdots,3; \quad n=1,\cdots,\infty \tag{23}$$

where λ_n denotes an eigenvalue and $\bar{\phi}_n$ denotes an eigenfunction. A direct computation of the solution of the above eigenvalue problem yields $\lambda_0 = 0$ with $\psi_0 = 1/\sqrt{2\pi}$, and $\lambda_n = \nu n^2 - \kappa n^4$ (λ_n is an eigenvalue of multiplicity two) with eigenfunctions $\phi_n = (1/\sqrt{\pi})\sin(nx)$ and $\psi_n = (1/\sqrt{\pi})\cos(nx)$ for $n = 1,\cdots,\infty$. Note that the $\bar{\phi}_n$ in Eq.23 denotes either ϕ_n or ψ_n. From the expression of the eigenvalues, it follows that for fixed values of $\nu > 0$ and $\kappa > 0$, the number of unstable eigenvalues of the operator A in Eq.23 is finite and the distance between two consecutive eigenvalues (i.e. λ_n and λ_{n+1}) increases as n increases.

We then derive nonlinear stochastic ODE formulations of Eq.21 using Galerkin's method. By substituting the expansion of $h(x,t)$ in terms of the eigenfunctions into Eq.21 and taking the inner product with the adjoint eigenfunctions, the following system of infinite nonlinear stochastic ODEs is obtained:

$$\begin{aligned}\frac{d\alpha_n}{dt} &= (\nu n^2 - \kappa n^4)\alpha_n + f_{n\alpha} + \sum_{i=1}^{p} b_{i\alpha_n}u_i(t) + \xi_\alpha^n(t)\\ \frac{d\beta_n}{dt} &= (\nu n^2 - \kappa n^4)\beta_n + f_{n\beta} + \sum_{i=1}^{p} b_{i\beta_n}u_i(t) + \xi_\beta^n(t)\end{aligned} \qquad n=1,\ldots,\infty \tag{24}$$

The control objective is the expected value of the surface roughness, r, which is modeled by the stochastic KSE and is represented by the standard deviation of the surface from its average height and is computed as follows:

$$\langle r(t)^2\rangle = \left\langle \frac{1}{2\pi}\int_{-\pi}^{\pi}[h(x,t)-\bar{h}(t)]^2dx \right\rangle \tag{25}$$

where $\bar{h}(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi}h(x,t)dx$ is the average surface height. The expected surface roughness, $\langle r(t)^2\rangle$ can be rewritten in terms of $\alpha_n(t)$ and $\beta_n(t)$ [17], [18]:

$$\langle r(t)^2\rangle = \frac{1}{2\pi}\sum_{i=1}^{\infty}\left[\langle\alpha_i(t)^2\rangle + \langle\beta_i(t)^2\rangle\right] \tag{26}$$

Therefore, the control problem of the expected surface roughness is equivalent to the state covariance control of the stochastic KSE. The proposed predictive control method can be applied to regulate the expected surface roughness.

2) Open-loop dynamics of the stochastic KSE: In the first simulation, we compute the expected value of open-loop surface roughness profile from the solution of the stochastic KSE of Eq.21 by setting $u_i(t) = 0$ for $i = 1,\cdots,p$. For $\nu = 1.975\times10^{-4}$ and $\kappa = 1.58\times10^{-4}$, the stochastic KSE possesses one positive eigenvalue. Therefore, the zero solution of the open-loop system is unstable. Surface roughness profiles obtained from 100 independent simulation runs using the same parameters are averaged and the resulting surface roughness profile is shown in Fig.1. The value of the open-loop surface roughness increases due to the open-loop instability of the zero solution. On the other hand, due to the existence of the nonlinear term, the open-loop surface roughness does not increase exponentially but it is bounded.

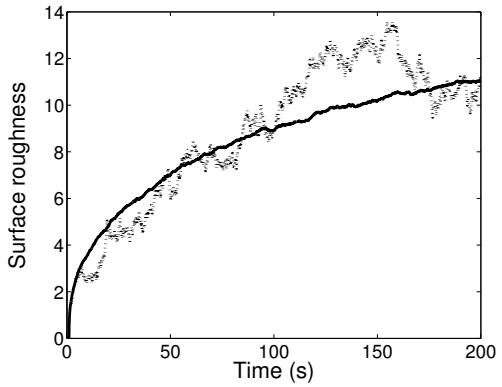

Fig. 1. The open-loop profile of the expected surface roughness resulting from the computation of the average of 100 independent simulation runs of the stochastic KSE of Eq.21.

3) Model reduction: Following the same way of model reduction of Eq.8, we rewrite the system of Eq.24 as follows:

$$\begin{aligned}\frac{dx_s}{dt} &= \Lambda_s x_s + f_s(x_s,x_f) + B_s u + \xi_s\\ \frac{dx_f}{dt} &= \Lambda_f x_f + f_f(x_s,x_f) + B_f u + \xi_f\end{aligned} \tag{27}$$

We note that the subsystem x_f in Eq.27 is infinite-dimensional. Neglecting the x_f subsystem, the following $2m$-dimensional system is obtained:

$$\frac{d\tilde{x}_s}{dt} = \Lambda_s\tilde{x}_s + f_s(\tilde{x}_s,0) + B_s u + \xi_s \tag{28}$$

where the tilde symbol in $\tilde{x}_s$ denotes that this state variable is associated with a finite-dimensional system.

4) Nonlinear predictive control of the stochastic KSE: In this closed-loop simulation, we design a predictive controller based on a $10th$ order stochastic ODE approximation constructed by using the first 10 eigenmodes of the system of Eq.21. Ten control actuators are used to control the system.

The ith actuator distribution function is taken to be:

$$b_i(z) = \begin{cases} \frac{1}{\sqrt{\pi}}\sin(iz); & i=1,\cdots,5 \\ \frac{1}{\sqrt{\pi}}\cos[(i-5)z]; & i=6,\cdots,10 \end{cases} \quad (29)$$

Under this control problem formulation, $m=5$ and the value of $\varepsilon = |\lambda_1|/|\lambda_{11}| = 4.21\times10^{-4}$. Our desired expected value of the surface roughness is 4.28. A reference trajectory for the expected surface roughness is constructed and is shown by the dotted line in Fig.2. The prediction horizon, T_p, of 180 s is selected, which is sufficiently large compare to the slow time scale in which the slow modes in the optimized closed-loop system evolves. Closed-loop simulations are performed to study the evolution of the expected value of the surface roughness under predictive control. To further simplify the computation, the predictive controller is solved by assuming that all the closed-loop poles of the finite-dimensional system are equal to each other. Closed-loop surface roughness profiles obtained from 100 independent simulation runs using the same simulation parameters are averaged and the resulting surface roughness profile is shown in Fig.2 (solid line) and it is compared with the open-loop surface roughness profile (dotted line). We can see that the controller successfully drives the surface roughness to the desired level, which is lower than that corresponding to open-loop operation ($u_i(t)=0$, $i=1,\ldots,10$).

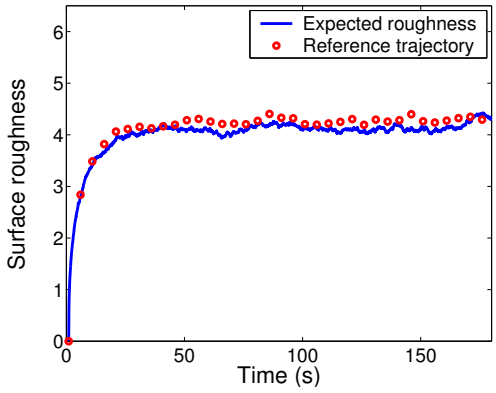

Fig. 2. The closed-loop profile of the expected value of the surface roughness of the nonlinear KSE under predictive control (solid line) vs. the reference trajectory.

5) Robustness properties of the predictive controller: In this subsection, we demonstrate the good robustness properties of the model predictive controller against parameter uncertainties of the stochastic KSE process model. To this end, we consider significant uncertainty in the parameters of the stochastic KSE process model. Specifically, the controller is designed based on the stochastic KSE model with the following parameters, $\nu_m = 1.975\times10^{-4}$, $\kappa_m = 1.58\times10^{-4}$, and $\lambda_m = 1.975\times10^{-4}$, where the subscript m denotes that the parameter is used by the model predictive controller design. However, the parameters of the stochastic KSE to which the predictive controller is applied are, $\nu = 1.5\nu_m$, $\kappa = 0.5\kappa_m$, and $\lambda = 1.2\lambda_m$, which correspond to a 50% uncertainty associated with ν and κ and a 20% uncertainty associated with λ. The proposed predictive controller is applied to the stochastic KSE model with the model uncertainties, and the simulation results are shown in Fig.3. It is clear that the predictive controller successfully regulates the expected surface roughness to desired level in the presence of significant model uncertainties.

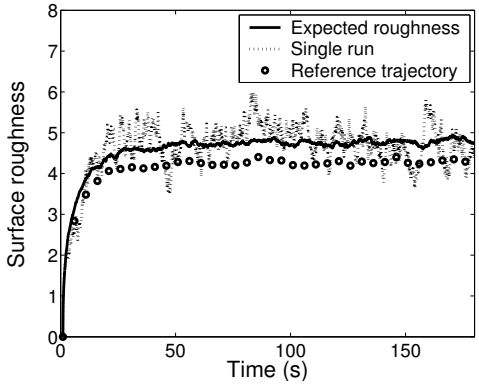

Fig. 3. The expected closed-loop surface roughness of the nonlinear KSE under the proposed predictive controller Effect of model uncertainty.

B. Model predictive control of an ion-sputtering process described by the stochastic KSE

Physical processes whose evolution of surface height can be modeled by the stochastic KSE, such as surface erosion by ion sputtering, can also be modeled by using kinetic Monte Carlo techniques (see, for example, [6], [16]). Since kinetic Monte Carlo models predict the evolution of surface roughness in these processes by directly simulating the formation of the surface under various surface micro-processes such as adsorption, desorption, surface erosion and surface reaction, kinetic Monte Carlo models have a higher accuracy for prediction of the surface roughness than the stochastic KSE model. To better verify the efficiency of the developed feedback controller, we implement linearization of the proposed nonlinear predictive controller to the kinetic Monte Carlo process model of a sputtering process [6] to control the surface roughness to a desired level.

1) Process description: We consider a 1-D-lattice representation of a crystalline surface in a sputtering process, which includes two surface micro-processes, erosion and diffusion. The solid-on-solid assumption is made which means that no defects or overhangs are allowed in the process. The microscopic rules are as follows: a site, i, is first randomly picked among the sites of the whole lattice and the particle at the top of this site is subject to: a) erosion with probability $0<f<1$, or b) diffusion with probability $1-f$.

If the particle at the top of site i is subject to erosion, the particle is removed from the site i with probability $P_e \cdot Y(\phi_i)$. P_e is determined as $\frac{1}{7}$ times the number of occupied sites in a box of size 3×3 centered at the site i, which is shown in Fig. 4. There is a total of 9 sites in the box. The central one is the

particle to be considered for erosion (the one marked by •). Among the remaining 8 sites, the site above the central site of interest must be vacant since the central site is a surface site. Therefore, only 7 of the 8 sites can be occupied and the maximum value of P_e is 1. $Y(\phi_i)$ is the sputtering yield function defined as follows:

$$Y(\phi_i) = y_0 + y_1\phi_i^2 + y_2\phi_i^4 \tag{30}$$

where y_0, y_1 and y_2 are process dependent constants and ϕ_i is the local slope defined as follows:

$$\phi_i = \tan^{-1}\left(\frac{h_{i+1} - h_{i-1}}{2a}\right) \tag{31}$$

where a is the lattice parameter and h_{i+1} and h_{i-1} are the values of surface height at sites $i+1$ and $i-1$, respectively.

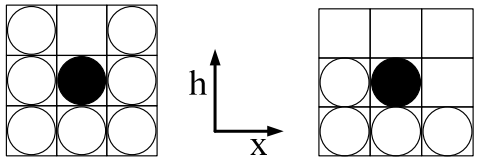

Fig. 4. Schematic of the rule to determine P_e. P_e is defined as $\frac{1}{7}$ times the number of occupied sites in a box of size 3×3 centered at the particle on the top of site i; $P_e = 1$ in the left figure and $P_e = \frac{4}{7}$ in the right figure, where the particle marked by • is on the top of site i.

If the particle at the top of site i is subject to diffusion, one of its two nearest neighbors, j ($j = i+1$ or $i-1$) is randomly chosen and the particle is moved to the nearest neighbor column with probability $w_{i\to j}$ as follows:

$$w_{i\to j} = \frac{1}{1+\exp(\beta\Delta H_{i\to j})} \tag{32}$$

where $\Delta H_{i\to j}$ is the energy difference between the final and initial states of the move, $\beta = \frac{1}{k_B T}$ and H is defined through the Hamiltonian of an unrestricted solid-on-solid model as follows:

$$H = \left(\frac{J}{a^2}\right)\sum_{k=1}^{L}(h_k - h_{k+1})^n \tag{33}$$

where J is the bond energy, L is the total number of sites in the lattice and n is a positive number. In the simulations presented in this paper, we use $n = 2$ and $\beta J = 2.0$.

The equation for the height fluctuations of the surface in this sputtering process was derived in [13] and is a stochastic Kuramoto-Sivashinsky equation of the form of Eq.34:

$$\frac{\partial h}{\partial t} = -\nu\frac{\partial^2 h}{\partial x^2} - \kappa\frac{\partial^4 h}{\partial x^4} + \frac{\lambda}{2}\left(\frac{\partial h}{\partial x}\right)^2 + \xi(x,t) \tag{34}$$

where $x \in [-\pi, \pi]$ is the spatial coordinate, t is the time, $h(x,t)$ is the height of the surface at position x and time t, ν and κ are two constants, and $\xi(x,t)$ is a Gaussian noise with zero mean and covariance:

$$\langle \xi(x,t)\xi(x',t')\rangle = \sigma^2\delta(x-x')\delta(t-t') \tag{35}$$

where σ is a constant, $\delta(\cdot)$ is the dirac function, and $\langle\cdot\rangle$ denotes the expected value. Note that the noise covariance depends on both space x and time t.

The parameters of the stochastic KSE model are identified by using a method reported in [12] as $\nu = 2.76\times 10^{-5}$, $\kappa = 1.54\times 10^{-7}$, $\lambda = 3.06\times 10^{-3}$, and $\sigma^2 = 1.78\times 10^{-5}$. Using the identified model parameters, the expected surface roughness predicted by the stochastic KSE model is consistent to that from the kMC model. However, there are observable model errors due to various approximations made in the process modeling procedures (see [12] for simulation results and detailed discussions). As demonstrated in the previous section, the proposed predictive controller is robust against significant model parameter uncertainties and is suitable to control the sputtering process based on an identified stochastic KSE process model.

2) Model predictive control of the sputtering process: In the closed-loop simulation, we design a predictive controller based on a $20th$ order stochastic ODE approximation constructed by using the first 20 eigenmodes of the system of Eq.34. First we design a linear state feedback controller as follows:

$$u(t) \;=\; \mathscr{B}_s^{-1}\{(\mathscr{A}_{cs}(t) - \mathscr{A}_s)\tilde{x}_s(t)\} \tag{36}$$

where $\mathscr{A}_{cs}(t) = diag[\lambda_{c1}(t)\ \cdots\ \lambda_{cm}(t)]$. $\lambda_{ci}(t)$ $(1 \le i \le m)$ are time-varying, desired poles of the closed-loop finite-dimensional system and the poles $\lambda_{ci}(t)$ are computed by solving the the optimization problem shown in Eq.14. Twenty control actuators are used to control the system. The ith actuator distribution function takes the same form as shown in Eq.29. Under this control problem formulation, $m = 10$ and the value of $\varepsilon = |\lambda_1|/|\lambda_{21}| = 0.02$. Our desired expected value of the surface roughness is 0.3. To further simplify the computation, the predictive controller is solved by assuming that all the closed-loop poles of the finite-dimensional system are equal to each other. Note that this predictive controller is the linearization around the zero solution of the predictive controller of Eqs.12 - 14.

Then, we apply the designed predictive controller to the kMC model of the sputtering process to control the surface roughness to the desired level. In this simulation, the initial surface roughness is about 0.5. The controller is implemented by manipulating the probability that a randomly selected site is subject to erosion rule, f. Specifically, the f of site i is determined according to the following expression:

$$f(i) = \frac{\bar{f} + \left(\sum_{j=1}^{20} b_j(z_i)u_j(t)\right)/a}{1 + \left(\sum_{j=1}^{20} b_j(z_i)u_j(t)\right)/a} \tag{37}$$

Closed-loop surface roughness profiles obtained from 100 independent simulation runs using the same simulation parameters are averaged and the resulting surface roughness profile is shown in Fig.5. We can see that the predictive controller successfully drives the surface roughness very close to the desired level.

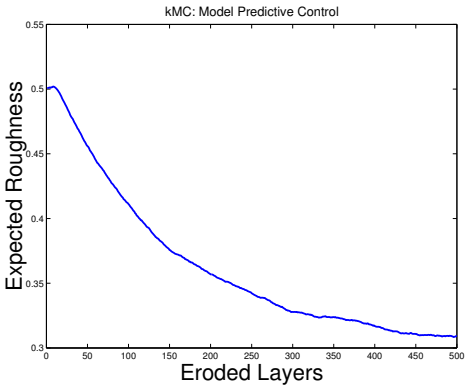

Fig. 5. The closed-loop profile of the expected value of the surface roughness under predictive control.

Remark 2: Note that although the stochastic KSE model of Eq.34 is a nonlinear model for the sputtering process, the linearization of the stochastic KSE around its zero solution is used to design the predictive controller of Eqs.36 and 14. This is made based on the following argument. Since the instability of the spatially uniform steady state comes from the linear part of the model, and the nonlinear part of the stochastic KSE helps bound the surface roughness, for control purposes, we only need to focus on the stabilization of the linear part of the stochastic KSE. This argument is further supported by our simulation results, which demonstrate the effectiveness of the predictive controller designed in this work.

V. Conclusions

We developed a method for model predictive control of nonlinear stochastic PDEs to regulate the state variance to a desired level. Initially, a system of infinite nonlinear stochastic ODEs is formulated from the nonlinear stochastic PDE by using Galerkin's method. To capture the dominant mode contribution, a finite-dimensional approximation was then derived. A model predictive control problem was formulated based on the approximation. This enabled computationally efficient prediction of state variance of the finite-dimensional system. The control action was computed by minimizing an objective penalty function. To characterize the closed-loop performance enforced by the model predictive controller, an analysis of the closed-loop nonlinear infinite-dimensional system was provided. The predictive controller was initially applied to the stochastic KSE and resulted in successful control of the norm of the state variance to a desired level in the presence of significant model parameter uncertainties. In addition, the problem of surface roughness regulation in a one-dimensional ion-sputtering process was considered. A model predictive controller was designed based on an identified stochastic KSE surface model to control the surface roughness of the sputtering process by manipulating the surface bombardment rate in a spatially distributed manner. The predictive controller successfully regulated the expected surface roughness to a desired level in the kMC model of the sputtering process.

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