239d Model Reduction, Estimation and Control of Multiscale Systems

Vinay Prasad

Multiscale systems offer unique challenges in modeling and control. From a modeling viewpoint, these systems are of very high dimension. Most of the systems have a stochastic component, resulting in noisy outputs. Additionally, their models are usually not in standard state space form, meaning that the application of advanced control strategies is not straightforward. The small number of measurements available also means that observability is an important issue in estimation and model identification in these systems. From a system analyst's viewpoint, another important characteristic is that the variables we wish to control (surface roughness, for example) are typically microscale quantities, while the possible manipulated variables (temperature, pressure, flows) act at the macroscale. This means that the model identification and estimation at the microscale cannot be neglected in developing a control strategy.

In this work, we present an approach to the dynamic analysis and control of multiscale systems that involves building reduced order models at the microscale, connecting them with macroscale models, and constructing estimators and controllers based on the reduced order models. Previous studies on control of multiscale systems have attempted to construct estimators and controllers using reduced order models, and the order reduction has been achieved by grouping probabilities [1] or by using a smaller lattice [2]. However, the model identification and reduction methods used in the current work differ from these methods.

We consider multiscale models of the form where kinetic Monte Carlo (KMC) models describe the microscale behavior, and deterministic continuum models using partial differential equations are used to model the macroscale. However, the model reduction methods we choose ensure that the choice of the form of the microscale model is theoretically not a constraint on the application of the method. We choose two example systems to demonstrate the method - a copper PVD process [3] and an epitaxial growth process [4]. The main features of the Cu PVD model, which along with the KMC algorithm is taken from Wang et al. [3], are the inclusion of events representing deposition, adatom diffusion, ledge adatom diffusion, dimer diffusion and diffusion across facets at the microscale. The epitaxial growth model, taken from Raimondeau and Vlachos [4], is also a KMC model and includes events describing adsorption, desorption and surface migration. Both of these models provide predictions of surface evolution at the microscale as a function of time. Consistent with previous treatments, the macroscale behavior in both systems is modeled as a stagnation-point flow reactor. The variables to be controlled in these systems are the growth rate and surface properties such as microroughness, and the manipulated variables are temperature and inlet mole fractions or fluxes.

The model reduction methods used in this work are of two types - proper orthogonal decomposition (POD) and a balanced truncation-type approach. Both methods use simulation data and system snapshots to construct the reduced order models. While the POD results for the epitaxial growth model matches those reported in [4] and [5] (i.e., low number of basis functions), the POD analysis for the Cu PVD system reveals the need for a much larger number of basis functions (approx. 25). Motivated by the application of nonlinear PCA methods with artificial neural networks (ANNs) [6] to KMC models and the results of Shvartsman et al. [7] in which slaving of higher pod modes (using ANNs) was found to be an efficient model reduction strategy for nonlinear distributed parameter systems, we apply a state-space model reduction method developed by Prasad and Bequette [8] to reduce the number of basis functions in the reduced order model. Since a POD analysis from snapshots only provides us with an input-output model and not an input-state-output model, we implement another model reduction method based on balanced truncation and compare the results with the POD-derived model. The nonlinear balanced truncation methods use empirical observability and controllability Gramians as described by

Lall et al. [9]. The reduced order microscale models are linked with the reactor scale models to derive the estimation and control algorithms.

The reduced order models described above are used in two different methods of identification and estimation. In the first case, we develop an estimator for the system using the reduced order models. The estimator is an extended Kalman filter, and is applied to both types of reduced order models. Unlike the results of Raimondeau and Vlachos [4], we find that direct interpolation of POD based models to intermediate conditions or parameter values (for example, interpolation using POD models developed at 200 and 400 C to a system at 300 C) does not provide good results. Consequently, we also develop a multiple model based identification approach to extend the use of the reduced order models to situations outside the phase space envelope for which they have been derived. This approach uses measurements to optimally blend models to obtain the best predictive model.

Finally, we design PID and model-based controllers based on the identified and estimated reduced order models and provide simulation results on the multiscale systems, which show the efficacy of the developed methods in controlling microscale properties like surface roughness.

References:

1. M.A. Gallivan, "Optimization, estimation and control for kinetic Monte Carlo simulations of thin film deposition", Proc. IEEE Conf. Decision Control, 3437-3442 (2003).

2. Y. Lou and P.G. Christofides, "Feedback control of growth rate and surface roughness in thin film growth", AIChE J., 49(8), 2099-2113 (2003).

3. Z. Wang, Y. Li and J.B. Adams, "Kinetic lattice Monte Carlo simulation of facet growth rate", Surf. Sci., 450, 51-63 (2000).

4. S. Raimondeau and D.G. Vlachos, "Low-Dimensional approximations of multiscale epitaxial growth models for microstructure control of materials", J. Comp. Phys., 160, 564-576 (2000).

5. M. A. Gallivan, R. M. Murray and D. G. Goodwin, "The dynamics of thin film growth: A modeling study", Proc. CVD XV (Electrochem. Soc.), 616, 168-175 (2000).

6. M.A. Gallivan, "Low-order dynamics in a lattice model of thin film deposition, using nonlinear principal component analysis", Proc. DYCOPS-7 (2004).

7. S.Y. Shvartsman, C. Theodoropoulos, R. Rico-Martinez, I.G. Kevrekidis, E.S. Titi and T.J. Mountziaris, "Order reduction for nonlinear dynamic models of distributed reacting systems", J. Proc. Control, 10, 177-184 (2000).

8. V. Prasad and B. W. Bequette, "Nonlinear system identification and model reduction using artificial neural networks", Computers Chem. Eng., 27 (12), 1741-1754 (2003).

9. S. Lall , J.E. Marsden and S. Glavaski, "A subspace approach to balanced truncation for model reduction of nonlinear control systems", Int. J. Robust Nonlinear Control, 12(5), 519-535 (2002).