503e Dynamic Optimization of Stochastic Systems Using in Situ Adaptive Tabulation

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In recent years there has been increased interest towards process optimization and control based on detailed process models both at macroscopic and microscopic length scales. For example, in the microelectronics industry, optimization and control strategies are being developed for thin-film deposition processes that utilize not only detailed nonlinear PDEs (derived from conservation laws), but also detailed kinetic Monte Carlo (kMC) or Molecular Dynamics (MD) based microscopic models, to achieve product quality objectives ranging from film thickness uniformity to microstructure. An ubiquitous roadblock, however, is the computational complexity of these models, which limits their applicability for optimization and control purposes. Consequently, considerable research effort is being devoted towards development of reduced, ``computationally friendly'', multiscale process models that capture the dominant traits of the detailed process descriptions across all relevant scales, yet allow swifter computation when implemented on a digital computer [1,3].

We present an extension of the multiscale optimization approach presented in [3] to dynamically evolving systems, restricting ourselves to microscopic domain of the multiscale process model. Specifically, we employ the in situ adaptive tabulation (ISAT) scheme in the context of kMC-based process descriptions to derive approximate multiscale integrators. The derived process integrators are employed towards the efficient solution of dynamic optimization problems using standard search algorithms. ISAT was originally developed in [2] for computationally efficient implementation of combustion chemistry through efficient ``on-demand'' tabulation of the process data and process sensitivities and speed-up factors of the order of 1000 were achieved. However, the underlying stochasticity prohibits direct application of ISAT to processes described by kMC simulations. In this work we outline conditions that guarantee unbiased and accurate estimation of process gradients with respect to initial conditions and process parameters for stochastic systems, thus formulating the basis for extending the applicability of ISAT to such systems. The motivation behind this approach is to circumvent repeated calculations of expensive time-steppers during optimization and simultaneously, whenever possible, utilize the sensitivity information to accurately interpolate process evolution from the tabulated database, without directly computing it from the time-stepper. In order to demonstrate the effectiveness of the proposed scheme, we consider two illustrative examples, namely, a stiff homogeneous chemically reacting system and a surface catalytic oxidation process. In both cases, we solve a dynamic optimization problem to compute optimal control trajectories that maximize pre-specified process objectives. Application of the ISAT algorithm during solution of the optimization problem resulted speed-up factors of about 100.

References

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