Microarray advances in the current computing capabilities have made it possible to investigate complex processes that were previously computationally intractable. Diverse fields benefit from these advances such as microelectronics and biomedical fields. Examples include from the microelectronics field the ever pressing demand for high performance devices which implies the allowable manufacturing tolerances are getting increasingly stringent, and from the biomedical field the need to design new drugs and identify efficient medication strategies.

Recent results in optimization algorithms have, in principle, made it possible to design complex processes that are optimal with respect to certain criteria. An underlying requirement is that a computationally tractable mathematical model capable of describing the dynamic evolution of the process with sufficient detail is available. For example, precise regulation of the performance of key industrial products is currently an important yet unresolved research problem with broad industrial implications. Such requirements necessitate the regulation of microscopic product properties within tight limits; this in turn requires the development and implementation of computationally-efficient model-based optimal operation and control policies on the processes that make the specific product. Similarly, treatment of HIV infection is an important challenge in today’s society. Current drugs merely prolong the life expectancy and enhance the quality of life of the patients; an important shortcoming of these drugs is their toxicity and can cause serious side effects, for instance liver failure. Consequently, quantification of drug toxicity effects, the probability of infection clearance and the computation of dosage strategies that are optimal with respect to quality of life is of vital importance.

Fundamental mathematical models that can accurately describe all the aspects of these processes are usually a combination of macroscopic/continuum models that describe the process bulk properties and microscopic/atomistic simulations that give the necessary accuracy when it is needed. These models are referred to as multiscale process systems and their solution requires very high computational requirements. Therefore, computationally-efficient techniques for the computation of high-performance operation and control policies should utilize highly-accurate, yet computationally tractable approximations. Motivated by this, the broad objective of our research is to resolve the fundamental issues associated with computing optimal operation and control policies for complex process systems. In this talk, I will present (a) the development of computationally-efficient algorithms for optimization and optimal operation of such processes and (b) the development of nonlinear, low-order, approximate models and construction of practically implementable feedback control systems that can deal with the issues of nonlinearity, model uncertainty and constraints. I will finally present applications of the presented methods towards (a) the optimal operation of a representative metal-organic vapor phase epitaxy process and (b) the identification of optimal medication schedules that maximize the probability of HIV infection clearance during the primary stage.