Numerical Simulation and Modelling of Electronic and Biochemical Systems

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Numerical Simulation and Modelling of Electronic and Biochemical Systems

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Abstract

Numerical simulation and modelling are witnessing a resurgence. Designing systems with integrated wireless components, mixed-signal blocks and nanoscale, multi-GHz "digital" circuits is requiring extensive low-level modelling and simulation. Analysis and design in non-electronic domains, notably in systems biology, are also relying increasingly on numerical computation.

Sections 2–8 of this Monograph provide an introduction to the fundamentals of numerical simulation, and to the basics of modelling electronic circuits and biochemical reactions. The focus is on a minimal set of concepts that will enable the reader to further explore the field independently. Differential–algebraic equation models of electronic circuits and biochemical reactions, together with basic numerical techniques — quiescent, transient and linear frequency domain analyses, as well as sensitivity and noise analyses — for solving these differential equations are developed. Downloadable MATLAB implementations are provided.

The last two chapters provide an introduction to computational methods for nonlinear periodic steady states and multi-time partial

differential equation (PDE) formulations, followed by an overview of model order reduction (MOR) and, at the end, a glimpse of some applications of oscillator MOR — in circuits (PLLs), biochemical reaction–diffusion systems and nanoelectronics.

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Introduction

1.1 Trends in Numerical Simulation and Applications

Since the advent of integrated circuits (ICs), numerical modelling and simulation have played an important rôle in analog, mixed-signal and RF design. Simulation is typically used to verify correctness and debug circuits during their design. Over the years, computer simulation has almost entirely replaced breadboarding and physical prototyping, especially for IC designs, where fabrication is expensive and time-consuming, and probing internal nodes difficult. Being able to "run" a circuit in simulation makes it much more likely to function correctly when it is actually built.

As a discipline, circuit simulation emerged in the late 1960s and early 1970s, with early programs like CANCER [70] maturing into design tools such as ASTAP [118] and SPICE [69, 89, 90]. These programs became popular during the chip design boom of the 1970s and enabled the design of new generations of ICs. After the early 1980s, simulation — the first electronic CAD discipline and arguably the progenitor of the electronic design automation (EDA) industry — became supplanted by other areas of EDA, such as physical design, combinatorial and sequential synthesis, formal verification, model checking, *etc.* However, the past decade has witnessed a resurgence in simulation and related areas (such as model-order reduction).

This resurgence has been spurred by several factors. Ever-shrinking DSM technologies have resulted in analog and digital designs both becoming markedly less ideal. Indeed, at lower levels of design, the distinction has become blurred, with continuous/analog effects being pervasive and causing digital abstractions to break down. This trend started almost three decades ago, when delay and crosstalk started becoming important concerns in digital design, first at the gate level and then in interconnect; today, huge chip sizes and extensive system-level integration — e.g., in systems-on-chip (SoCs) and systems-in-packages (SiPs) — have made interference and noise crucial limiting factors in virtually all digital and mixed-signal designs. Moreover, as feature sizes have evolved toward the 22 nm node over the last decade, low-level non-ideality in transistor characteristics has emerged as another serious design issue. An important aspect of this non-ideality is greatly increased parameter variability. These effects are all continuous, or analog, in nature, hence call for low-level simulation and modeling tools during design and verification.

Integrated RF and communication system design, which since the mid-1990s has constituted an important part of the semiconductor industry's portfolio, has been another driver for numerical simulation and modelling. Such designs involve analog/mixed-signal, RF and digital components on the same substrate.

They also frequently involve micro/nanoelectromechanical system (MEMS/NEMS) elements and electromagnetic (EM) structures, such as antennas and transmission lines; and, to a lesser extent, optical and even biological elements. These trends have increased reliance on simulation technologies, not only during the design of individual circuits, but for the verification of larger systems. Indeed, interactions between analog/mixed-signal, RF, non-electronic and digital systems are a prolific source of design problems and functional failures; an important use of low-level simulation and modelling tools is to help debug such problems.

It is for these reasons that numerical simulation and modelling have been growing in importance and seeing steadily increasing practical application. The proliferation of physical domains for which simulation technologies are now needed, compounded by generally increased complexity, has expanded the scope of numerical simulation and modelling within CAD and spurred new research directions. For example, interconnect issues drove research in EM simulation and extraction, and in linear model-order reduction (MOR), through the 1990s. Efficient algorithms for periodic and stochastic (noise) analysis of large nonlinear circuits and systems, developed in the mid to late 1990s, were driven by the integrated RF ICs which fueled the portable wireless revolution. Nonlinear stochastic simulation, currently a topic of active research, is motivated by the parameter variability problem. Automated nonlinear computational macromodelling, or nonlinear MOR, is similarly a topic of current interest because it enables system level verification and design. The rise of multi-core computational platforms has led to parallelization of numerical simulation algorithms becoming yet another topic of current interest.

Another exciting driver for research in the above areas is biological systems. The past decade has witnessed tremendous progress in mathematical biology; biology has been transforming into a precise, quantitative, bottom-up, predictive discipline, much as physics and engineering did over the last century. Even more than in electronics, biological systems feature many individual entities that interact extensively and are organized hierarchically, with logical functionality emerging from the hybrid interplay of discrete and continuous-time dynamics; and to a much greater extent than the human-engineered systems of today, understanding how most biological systems work — even qualitatively — is often simply not possible at all without computational tools. Similar circumstances led to CAD tools becoming indispensable in electronics. The same is happening in the biological arena; effective leveraging of computational techniques from electronics and engineering systems can catalyze progress in the field.

1.2 Scope and Organization of This Monograph

This Monograph provides an introduction to the fundamentals of numerical simulation, and to the basics of modelling electronic circuits and biochemical reactions. The emphasis is on capturing a minimal set of important concepts succinctly, but concretely enough that the reader will be left with an adequate foundation for further independent exploration. Starting from mathematical models of basic electronic elements, circuits are modeled as nonlinear differential–algebraic equation (DAE) systems. Two basic techniques — quiescent steady state and transient — for solving these differential equations systems are then developed. It is then shown how biochemical reactions can also be modeled deterministically as DAEs (hence simulated using the various numerical simulation methods developed of this Monograph). Following this, frequency domain techniques for finding sinusoidal steady states of linear DAEs are developed, as are direct and adjoint techniques for computing parameter sensitivities and the effects of stationary random noise.

For readers interested in a glimpse of topics beyond these basics, an introduction to nonlinear periodic steady state methods (harmonic balance and shooting) and the multitime partial differential equation formulation is provided. Also provided is an overview of model order reduction, an important topic of current research that has roots in numerical simulation algorithms. Finally, sample applications of nonlinear oscillator macromodels — in circuits (PLLs), biochemical reaction–diffusion systems and nanoelectronics — are presented.

1.3 Website for MATLAB Scripts and Updates

The reader is encouraged to visit the following URL, which contains MATLAB implementations illustrating topics in this Monograph:

http://www.eecs.berkeley.edu/∼jr/NOW-FT-Monograph/.

The site also contains addenda and updates.

1.4 Acknowledgments

The basic material in the earlier chapters of this Monograph is strongly influenced by [7]. The author would like to acknowledge a number of distinguished colleagues for contributing materially to his knowledge of the topics in this Monograph: Raj Raghuram, Bob Brayton, Peter Feldmann, Alper Demir, Amit Mehrotra, Joel Phillips, Onuttom Narayan, Hans-Georg Brachtendorf, David Long, Bob Melville and Jacob White. Much of the material on applications of nonlinear oscillator macromodels is the work of Xiaolue Lai; results from piecewise polynomial trajectory-based nonlinear macromodelling are the work of Ning Dong. The author thanks Sharad Malik and James Finlay for their patience and helpfulness during the development of this Monograph.

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