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PREFACE

A fundamental challenge in engineering, physical and life sciences is the quantitative prediction of time-dependent phenomena governed by ordinary differential equations (ODEs). While simulation of ballistic trajectories was one of the very first applications of digital computers, numerous more demanding ones have emerged, calling for new numerical schemes and improved implementations. In molecular dynamics, astronomy, chemistry, robotics or optimal control for instance, numerical simulation can often replace real experiments that are impossible or too expensive to carry out.

In recent years, the field of numerical integration has seen some very noticeable theoretical developments: research groups worldwide have brought to the fore new fundamental concepts and techniques, such as, for instance, Butcher series, backward error analysis, modulated Fourier expansions..., which altogether have led to a deeper and wider understanding of the behavior of numerical methods for ODEs at large, and for special classes thereof in particular (Hamiltonian systems, ODEs on manifolds or in Lie-groups, highly-oscillatory problems...). The effort is now gradually shifting to other types of equations (stochastic ODEs, conservative PDEs...) for which the techniques developed in the ODE context are expected to bring some new light.

At the same time, advances in engineering, physical and life sciences in understanding and manipulating physical phenomena at the micro and nanoscales have demanded a new technology for modeling, simulation and analysis of experimental and simulation results which can handle heterogeneous models at multiple scales. Both theory and practice in numerical integration is playing a fundamental role in many new application arenas.

This special issue of *ESAIM: M2AN* is an attempt to witness this trend: it collects twelve contributions covering a very broad spectrum of techniques and types of differential equations, from purely algebraic tools to long-time error estimates, from Newton's equations to Schrödinger's equation, inspired by applications ranging from electronics to physical therapy. It answers the desire of the Editors-in-Chief C. Le Bris and A.T. Patera to expose an important and active field which appears somewhat underrepresented within the *ESAIM: M2AN* readership and authorship.

The issue opens with a paper by P. Chartier and A. Murua, which is a follow-up of several recent articles devoted to a structure appearing in numerical integration and called *Hopf algebra*. It presents an abstract framework describing algebraically the derivation of order conditions irrespective of the nature of the ODE considered or of the type of integrator used.

The next two papers are concerned with *geometric* properties of integration schemes and are representative of what is known as *geometric numerical integration*. The first, by E. Hairer, R.I. McLachlan and R.D. Skeel deals with the simplified Takahashi-Imada method (a modification of the Störmer-Verlet method) which is symmetric and volume-preserving but no longer symplectic. The possibility of an energy-drift for this method is supported both theoretically and experimentally, emphasizing the importance of using a symplectic integrator for molecular dynamics simulations. The second, by E. Celledoni, R.I. McLachlan, B. Owren, G.R.W. Quispel and W. Wright, focuses on Runge-Kutta methods preserving energy in Hamiltonian systems. The proposed construction relies on the Average Vector Field method recently introduced by two of the present authors.

Another pair of articles is devoted to conservative schemes for the Schrödinger equation. The first, by F. Castella and G. Dujardin, considers splitting methods for the linear case and extends previous results by E. Faou and G. Dujardin to the situation where less regularity on the initial conditions is required. The second, by M. Dahlby and B. Owren, is concerned with the case of a cubic potential and analyses the plane wave stability of two numerical methods introduced respectively by C. Besse and by Z. Fei. An extension of the latter that is more stable is also presented.

Numerical ODE technologies play an important role in the solution of other classes of numerical problems, as demonstrated in the following two papers. The paper by U.M. Ascher, K. van den Doel, H. Huang and B.F. Svaiter proposes stepsize selection strategies to accelerate the convergence of PDE methods to a steady state solution. The paper by M. Hochbruck, M. Hönig and A. Ostermann considers a regularization technique for ill-posed nonlinear problems based on the numerical solution of an ODE (Showalter ODE). It is shown that the use of a variant of the exponential Euler method, rather than merely the Euler method, when combined with Krylov-space techniques, improves the efficiency.

The problem of simulating molecular dynamics over physically meaningful time scales has inspired many new algorithms and results in numerical integration and analysis of simulation trajectories. The paper by C. Schütte and T. Jahnke introduces a new method for approximating the effective dynamics of a system (for example, folding of proteins) which switches between metastable states only rarely. The paper by B. Leimkuhler and S. Reich deals with molecular dynamics under constant temperature. Focusing on the Nose-Hoover thermostat technique, they demonstrate that the method respects detailed balance.

The paper by A. Zagaris, C.W. Gear, T.J. Kaper and I.G. Kevrekidis deals with an important issue for multiscale simulation in a more general context: development and analysis of iterative algorithms within the context of equation-free methods to approximate low-dimensional, attracting, slow manifolds in systems of differential equations with multiple scales.

Simulation of electronic circuits has long been an important application driving the development of new numerical integration technologies. This continues to be the case. The recent explosion of developments in the Radio Frequency (RF) and telecommunications industry, faster designs and faster product output, for smaller and smaller components where resolution of crosstalk issues can require a multiscale treatment. The paper by M. Condon, A. Deano and A. Iserles focuses on highly oscillatory ODEs arising in RF communication systems, and proposes a new time-stepping method that guarantees high accuracy for linear ODE systems regardless of the rate of oscillation.

The final paper deals with oscillations in a completely different realm: tissue modeling. It is known that healthy skeletal muscle cells oscillate at a specific frequency, whereas unhealthy muscle cells, and muscle cells in outer space missions (which rapidly become unhealthy) don't. The paper of B. Simeon, R. Serban and L.R. Petzold explores *via* mathematical model the physical pnenomenon of microvibration of skeletal muscle cells, and how these oscillations can be entrained by an externally applied vibration used in a type of physical therapy. The resulting partial differential-algebraic equation model presents challenges for the numerical solution. The modeling results suggest some possible explanations for the effectiveness of the therapy.

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