EDUCATION

This issue of *SIAM Review* presents two papers in the Education section. The first paper, "Time Correlation Functions of Equilibrium and Nonequilibrium Langevin Dynamics: Derivations and Numerics Using Random Numbers," is coauthored by Xiaocheng Shang and Martin Kröger. Langevin dynamics is a term describing a mathematical model of the dynamics of molecular systems which uses stochastic differential equations. This model extends the molecular dynamics to allow for describing effects due to friction caused by solvent or air molecules or other phenomena that perturb the system. In this paper, the authors present the model equation for the behavior of a harmonic oscillator in two or three dimensions in the presence of friction, additive noise, and an external field with both rotational and deformational components. They study the time correlation function of the dynamics analytically and numerically. The paper provides a good illustration of the tools of stochastic calculus on a nontrivial application and helps evaluate the numerical solvers for stochastic differential equations (SDEs).

The authors argue that the fair assessment of the efficiency and accuracy of numerical solvers for SDEs requires access to analytical reference solutions. However, deriving relevant analytical formulae is possible only for very simple cases. Here a two-dimensional nontrivial benchmark problem is analyzed and an exact solution is derived. The analysis in the paper includes also a discussion on inertial effects. The model equation formulated in section 2 is interesting because it arises in multiple applications. Furthermore, the absence of the restoring force or the external field in the model leads to popular special cases. Among those are the random walk, diffusion models, the motion of atoms in the presence of gravitational or centrifugal potential, nanomagnets subjected to magnetic fields, Brownian oscillators, rotational relaxation of molecules trapped in a three-dimensional crystal, and many others. Relevant literature describing those models is provided. The authors describe a direct approach to the derivation of the time correlation functions for general Langevin dynamics, as well as an approach that uses Fourier transforms and the Wiener–Khinchin theorem, and a complementary approach via the associated Fokker–Planck equation. The last portion of the paper contains the description of two numerical methods and numerical experience.

The second paper presents "An Introduction to Quantum Computing, without the Physics," written by Giacomo Nannicini. This paper introduces discrete mathematicians and computer scientists to quantum computing. While quantum computing uses certain quantum phenomena to perform computation, many scientists may learn about its principles without acquiring deeper knowledge of quantum physics.

The author starts with a set of assumptions that are satisfied by a quantum computing device. From those assumptions further properties are derived in a rigorous way. The necessary concepts are formally introduced and all statements are supplied with mathematical proofs. The author adopts a model of computation, which is known as the quantum circuit model. Quoting from the paper, it works as follows:

1. The quantum computer has a state that is contained in a quantum register and is initialized in a predefined way.
2. The state evolves by applying operations specified in advance in the form of an algorithm.
3. At the end of the computation, some information on the state of the quantum register is obtained by means of a special operation, called a measurement.

At the beginning of the paper, some properties of the tensor product are reviewed, which are used to express states and operations in a quantum device. For example, qubits are the quantum counterparts of the bits in our computers and the

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state of a q-qubit quantum register is identified with a unit vector in the space $(\mathbb{C}^2)^{\otimes q}$, where $\mathbb{C}^2$ is the complex Euclidean space. The exposition proceeds with the introduction and analysis of the types of states and their properties, the quantum phenomena of superposition and enlargement, measurement gates, and the input-output model for quantum computations. The second portion of the paper discusses several quantum algorithms including a numerical implementation of Grover's algorithm. It may be of interest that, although quantum computing is able to solve some problems much faster than the classical computer, it is still not known to solve NP-complete problems efficiently. The paper concludes with a section containing notes for further reading.

According to the author's experience, the paper provides material for a graduate-level module in quantum computing for mathematicians and computer scientists. It is recommended to split the material into five lectures/meetings of 90–120 minutes each. The last meeting would aim at providing a hands-on numerical experience based on section 6 of the paper. The audience should be familiar with linear algebra and with basic concepts in computing such as Turing machines and algorithmic complexity.

Darinka Dentcheva
Section Editor
darinka.dentcheva@stevens.edu