

We might ask, If one has the attention of young chemistry-oriented students for one semester, is this a good introduction to the subject? Quantum mechanical calculations are now firmly established as an everyday tool in the chemistry laboratory, especially for molecular geometries (conformational analysis), energy levels (spectroscopy), properties (dipole moments, polarizabilities), heats of reaction and equilibria (thermochemistry), and reaction mechanics (reactive barrier heights and thermochemical kinetics). Furthermore, chemists need to understand the conceptual framework of quantum mechanics, especially discreteness, uncertainty, coherence, interference, orbital symmetry, and tunneling. How well does the present text succeed in preparing students to appreciate the quantum mechanical concepts underlying modern calculations and interpretations of chemical phenomena?

In my opinion the book is well done in a limited number of these areas but is deficient in that it does not provide a broad enough view. For example, a point in favor of the book is that the critical Born–Oppenheimer separation of electronic and nuclear motion is explained, but a weak point is that the author does not address some important questions: How good is the Born–Oppenheimer approximation as a quantitative method for normal molecules? (Very good indeed.) Or when do we need to go beyond this approximation? (For photochemistry, for example.)

Consider another example: harmonic vibrations and normal coordinates. Normal coordinates are explained in words, without derivation, which is a reasonable compromise for beginning students. Furthermore, the example of internal rotation (torsion) is provided, and the students can see a case in which the harmonic approximation breaks down. But the internal rotation problem is presented only in the context of rotations, and its relation to the harmonic approximation is not presented.

The author presents the self-consistent field (SCF) method for atoms but does not tie it in to the early chapters, in which the variational principle is presented; the student might not realize that the SCF method is an example of the variational method. The comparison between the configuration interaction method and perturbation theory for treating electronic correlation is too oversimplified to be helpful.

The treatment of electronic structure is the strongest part of the book, especially in that the author intro-

duces molecular mechanics, semiempirical molecular orbital theory, solvation effects, and density functional theory (DFT), although all at a very introductory level. The discussion of DFT gives the impression that one can systematically optimize the exchange–correlation density functionals until they converge “closer and closer” to the correct result, but this is not true. The author also errs in stating that including solvation is formidable; this is not true either. Only one paragraph is devoted to transition states, and it is drastically inadequate.

In my opinion the text is too simplified and restricted in scope to be a good choice for introducing students to quantum chemistry. It does not provide the student with an adequate understanding of the fundamentals and concepts.

DONALD G. TRUHLAR
University of Minnesota
Minneapolis

Inviscid Incompressible Flow

▶ Jeffrey S. Marshall
Wiley, New York, 2001. \$90.00
(378 pp.). ISBN 0-471-37566-7

Jeffrey S. Marshall's *Inviscid Incompressible Flow* is a refreshing compendium of classical topics in the repertoire of fluid dynamists, physicists, and mathematicians. It also contains some computational tools that a current student and practitioner of inviscid fluid dynamics must have. The author, who works in continuum mechanics, has been active in both theoretical and computational mechanics—hence a book with a viewpoint, and perhaps some coloration, which reflects his personal experience. The motivation for the book is the success of the inviscid flow formulation in describing the behavior of fluids as we ordinarily encounter them—in breathing, or flying, or experiencing the interplay of oceanic and atmospheric currents.

In Marshall's book, the fluid flow problem is formulated first in integral and then in differential form, after the reader is carefully guided through a series of mathematical and kinematical preliminaries needed for rigorous deductions from the conservation laws of mechanics. The formulation is completed with a chapter-long discussion of interfaces. Marshall next discusses the general conclusions regarding the global features of flows in terms of velocity, vorticity, and pressure theorems. The bulk of the discussions of flows is nearly equally

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divided between potential flows and vortical flows in chapters dispersed throughout the text. The book's final two chapters are on interfacial waves and flow instabilities.

Given that ample computing capacity has now become the norm, the book provides some computational tools needed to break free of classical analytical techniques and employ instead numerical calculations for the study of flows. This computational aspect is particularly suitable for instruction at universities where computational proficiency is expected of both undergraduate and graduate students.

Marshall's presentation of mathematical preliminaries prior to the formulation of problems is rigorous, which reflects his training in continuum mechanics; a novice might find his approach somewhat overpowering.

Although Marshall's discussion of the requirements for incompressibility is meticulous, a parallel presentation of the inviscid flow assumption, which would have made the discussion more thorough, is missing. Further, the last two chapters, on waves and instability, seem not to cover their material at the level comparable to, say, the coverage of vortex dynamics in earlier chapters. And some inclusion of observations and experiments would have been valuable to experimentalists like me; after all, it is the experiments that guide us.

Nonetheless, Marshall's book fills an important gap. It provides a rigorous formulation of the fluid flow problem and presents a compendium of fundamentally and technically important problems in inviscid incompressible flow. Additionally, it poses problems at the end of each chapter that can be used to further explore the preceding topics. An important achievement of the book from my point of view is that so much is done in a volume of reasonable size. Not a trivial task!

Even though the author sees *Inviscid Incompressible Flows* as a textbook for graduate-level teaching, I also envision it as a textbook for advanced undergraduate teaching in physics, mathematics, and engineering, as well as a complementary reference book for graduate courses in fluid mechanics. I certainly welcome the book as a nice addition to my own collection. In particular, I find the treatment of vortex filaments and vortex panel methods very useful, since I discuss those topics in the senior and first-year graduate courses I teach at Berkeley.

ÖMER SAVAS
University of California
Berkeley

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