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EDITOR'S CORNER

Herman Berendsen: Researcher, Teacher, Scholar, Colleague, Skipper

On September 30, 1999, Herman J.C. Berendsen will follow Dutch law and, at age 65, relinquish the chair for physical chemistry at the University of Groningen, The Netherlands, which he has held since 1967. This special issue is a tribute to his important role in the development of computer simulations of molecular dynamics, especially of biomolecular systems. Since he has served as associate editor of the journal Proteins: Structure, Function, and Genetics from its inception in 1986 until 1992, and has here published on average more than one paper per year. We have thought it fitting to invite contributions by researchers who have participated in collaborative research with Herman or in CECAM (Centre Européen de Calcul Atomique et Moléculaire) workshops organized by him over a period of more than 25 years, and who have contributed significantly to the research literature on biomolecular simulation. Seventeen manuscripts have been received and constitute this volume. It is truly a great pleasure to present this special issue in his honor.

Herman Berendsen studied experimental physics with majors in medical, technical and mathematical physics at the University of Utrecht, and then did his two years (1957–1959) of obligatory military service as officer in the Royal Dutch Navy. This in turn became the origin of a series of legendary sailing trips around Europe with yachts of the naval yacht club, which he skippered and shared with many of his coworkers and colleagues. From1959 until 1961, Herman was research associate in the neurophysiology group of the Research Laboratory of Electronics of the Massachusetts Institute of Technology, Cambridge, MA, where he was introduced to the emerging nuclear magnetic resonance (NMR) technique. His Ph.D. thesis, "An NMR study of collagen hydration," brought him a doctorate at the University of Groningen in 1962 and first illustrates his love for water at the microscopic level. The University of Groningen recognized Hermans great talents and appointed him associate professor in 1963 and full professor in 1967. Those were times when scientific and educational accomplishments were not yet measured using statistical indices: by 1963, Herman had published three papers and by 1967 his publication list had tripled to nine.

His early research centered around NMR of biologically relevant systems and water. Herman was one of the first to apply the NMR technique to biomolecular systems[1] thereby becoming one of a small group who stood at the cradle of this most fruitful application area. Herman's work on the interpretation of sodium NMR spectra in tissue was a second salient contribution to the development of biomolecular NMR.[2,3] His most beautiful and far reaching contribution in this area concerns spin diffusion in proteins, which has turned out to be of essential importance for a correct interpretation of two-dimensional NMR spectra of biomolecules.[4]

Computer simulation of biomolecules in particular proteins is a second area in which Herman has made essential contributions, and indeed has, with a handful of others, given its present shape. Milestones are his SHAKE method to perform molecular dynamics simulation in Cartesian coordinates with constraints,[5] one of the most widely used water models, namely, the simple (three-) point-charge (SPC) model for liquid water,[6,7] his pioneering study of free energy perturbation methods for computing hydration free energy via simulation,[8] the Berendsen thermostat and manostat for simulation at constant temperature and pressure,[9] and his density matrix evolution method for hybrid quantum/classical dynamics simulation.[10] The simulation of membranes was pioneered by the Berendsen group in the early eighties.[11–13] In addition to the development of methodology and the application of computer simulation, the construction of fast, efficient hardware to enable biomolecular simulations of relevant length has continuously had Hermans attention and interest.[14,15] Herman's current list of more than 230 papers, the most recent overwhelmingly on computer simulation of complex molecular systems of biological relevance[16] as well as numerous related publications by others, attest to the maturity of the field that he has helped found.

Herman Berendsen represents the best academic tradition of probing the unknown, of seeking both new knowledge and new and improved methods, but always with an eye to possible practical application. In this endeavor he has never hesitated to share his insights, knowledge, and ideas with others, as is best illustrated by the series of 13 CECAM workshops and discussion meetings he has organized and led since 1972. His scientific work is above all characterized by an exceptional scope, from mathematics, computer science, and physics to chemistry, biochemistry, molecular biology, and medical applications, and by a clear vision and foresight.

Herman's great didactic qualities and contagious enthusiasm have been and continue to be a great stimulus for

the over 80 students, postdocs, and visiting scientists who have studied or are now studying with him in Groningen. He has also done his share towards maintaining the scientific community, as editor of different journals, a member of a variety of national and international committees, and as president of IUPAB, to mention a few.

We hope and trust that Herman Berendsen will, after his official retirement, stay active as a role model for students and researchers, and that he will continue to contribute to our knowledge and understanding of dynamic biological systems. As editors of this volume, we have the special privilege of here expressing our personal debt to Herman as a colleague, teacher, and friend.

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