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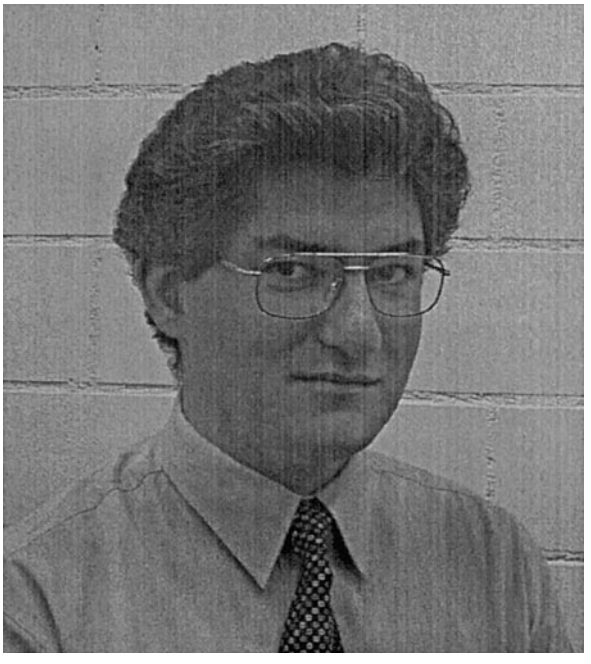
ANNOUNCEMENT
Paper of the Year Award

Congratulations to Ilya Reviakine and Willy Wriggers, co-recipients of the first Paper of the Year Award.

"Growth of Protein 2-D Crystals on Supported Planar Lipid Bilayers Imaged *in Situ* by AFM," by Ilya Reviakine, Wilma Bergsma-Schutter, and Alain Brisson, pp. 356–361 Volume **121,** No. 3, January 1, 1998 (doi:10.1006/jsbi.1998.4003).



Ilya Reviakine
University of Groningen

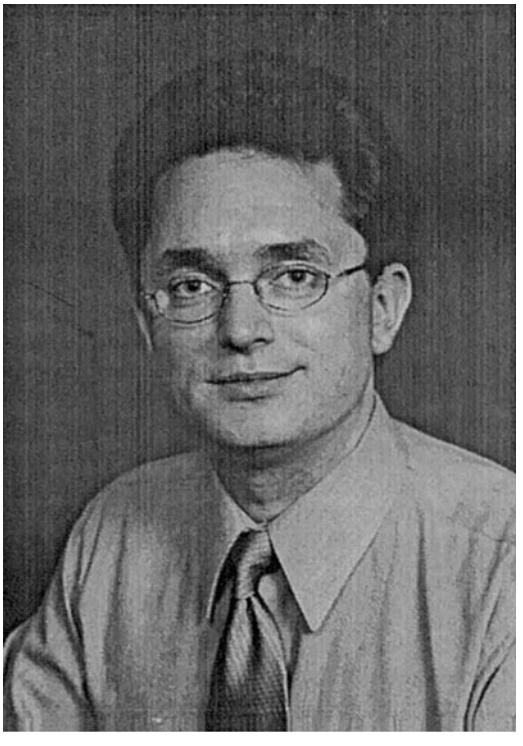
The *JSB* paper by Reviakine *et al.* reports on the formation of protein 2-D crystals on solid-supported lipid bilayers (SPBs), followed by atomic force microscopy. This work was performed by Ilya Reviakine, the Ph.D. student who initiated the AFM studies in our group in Groningen. For researchers devoted to crystallizing proteins, the main breakthrough from this paper is that the growth of protein crystals in 2D could be observed *in situ,* allowing direct evaluation of the influence of experimental parameters on crystal formation. The ability to image complex molecular processes in aqueous solutions at submolecular resolution offered by AFM was instrumental in the development of this technology. The mere observation of molecular processes inaccessible until now significantly improved our understanding of the crystallization process.

Some results presented in the *JSB* paper are likely to be of general relevance, such as the parallelism observed between lipid bilayers at a solid–liquid interface and lipid monolayers at an air–water interface as supports of protein 2D crystallization, the fact that crystallization proceeds via nucleation and crystal growth, and the presence of defects in 2D crystals.

Another area of research that has already benefited from this work is the formation of SPBs by vesicle fusion (I. Reviakine and A. Brisson, *Langmuir* **16,** 2000, 1806–1815), with its potential use in designing biocompatible surfaces. For annexin V, the protein system investigated in this paper, the AFM approach proved to be ideal for revealing the details of a transition between two 2D crystal phases, with p6 and p3 symmetry, respectively (I. Reviakine *et al., Langmuir,* in press).

The *JSB* paper provides the foundations of future technologies using solid-supported crystalline protein matrices for anchoring and immobilizing other elements, from proteins to nanoparticles, with exciting possibilities from structural biology to nanotechnology.

"Situs: A Package for Docking Crystal Structures into Low-Resolution Maps from Electron Microscopy," by Willy Wriggers, Ronald A. Milligan, and J. Andrew McCammon, pp. 185–195 Volume **125,** No. 2/3, April/May 1999 (doi:10.1006/jsbi.1998.4080).



Willy Wriggers
Scripps Research Institute

As a graduate student in the Department of Physics at the University of Illinois, Willy Wriggers received rigorous training in theoretical biophysics. In

Klaus Schulten's group he learnt some of the essential tools used in the computational analysis of biomolecular activity, and he extended and applied these to clarify issues related to molecular motor proteins, among others. Wriggers' early publications span the range from careful applications of molecular dynamics simulations in the analysis of the activity of cell motility proteins to the development of methods for simulating and mathematically characterizing large-scale conformational changes in proteins. During this time, he also developed neural computing methods that were under investigation in the Schulten group and in other groups at UIUC's Beckman Institute, and he configured artificial neural networks for biomolecular docking.

Wriggers' postdoctoral tenure at UCSD and TSRI provided him the opportunity to broaden his technical experience in new directions. Supported by *La Jolla Interfaces in Science* postdoctoral co-mentors Andy McCammon (UCSD) and Ron Milligan (Scripps), Wriggers developed information processing strategies for modeling 3D structures of macromolecules at various levels of resolution. The underlying methods were tested at UCSD and applied to experimental data at Scripps. The development in recent years toward the study of large macromolecular aggregates with EM provide a basis for the combination of multiscale biophysical data across a wide range of resolutions. The widening of Wriggers' research focus relative to his earlier training in physics and atomic modeling was therefore very timely.

Through Wriggers' association with Milligan's lab, he identified the need for a program to routinely dock atomic structures of single molecules to low-resolution EM data and then wrote a program package, Situs, to carry this out. The package makes use of single-molecule EM density maps that can be obtained by difference mapping using data from specimens of variable subunit composition. The main innovation of Situs was a reduced neural-network-based characterization of 3D data that enables users to correlate features within the structural data sets. The encoding of the data by a discrete set of point "landmarks" allows rapid docking of atomic structures into 3D EM maps. Though only released recently, the package has already received considerable attention in the EM community; the work was presented at the 1999 Gordon conference and 100 users have since registered the download. Consequently, a growing number of research groups use the software for their published work. The early versions of Situs were limited to rigid-body docking of single molecules, but recent advances allow flexible fitting of fully connected domains. Also, the modular nature of the package supports the inclusion of template convolution tools suitable for docking of subunits into entire aggregates.

Wriggers was appointed assistant professor in the Department of Molecular Biology at Scripps in 1999. His research program—to develop and disseminate fitting tools for electron microscopic data—is supported by grants from the National Institutes of Health.