

Frank Reidy Research Center for Bioelectrics Seminar Series

Multiscale Computational Modeling - From Atoms to Living Organisms

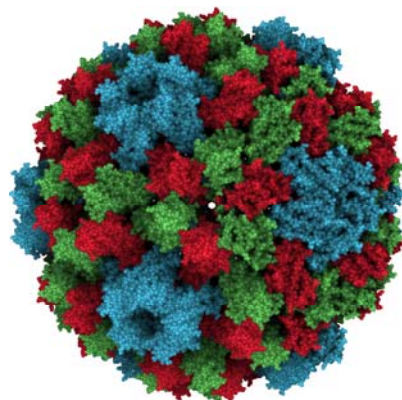
Speaker: Willy Wriggers, Ph.D.
Frank Batten Professor of Mechanical
and Aerospace Engineering Program
in Biomedical Engineering,
Old Dominion University



When: 9:00 AM, Tuesday, February 23, 2016
Where: 1st floor conference room, IRP II

Abstract:

As observed in long-timescale molecular dynamics simulations or in multi-scale 3D models, the behavior of “biological machines” that emerges on these temporal and spatial scales is not only more than the sum of the parts, but quite different and unexpected. Examples include: (1) slow conformational changes in protein folding and protein-protein binding enabled by fast motion in long molecular dynamics simulations; (2) the complex arrangement of the molecular building blocks of living organisms in low-resolution data from electron microscopy or tomography. I will argue that it may be useful to employ a “systems” perspective in computational biomolecular modeling whenever complex phenomena arise that cannot be predicted from isolated degrees of freedom.



Biosketch:

Dr. Wriggers earned a Ph.D. in Physics from the University of Illinois, Urbana-Champaign in 1998. He held postdoctoral positions in Electron Microscopy (Scripps Research Institute) as well as Theoretical Chemistry (University of California, San Diego). In 1999 he was appointed Assistant Professor at The Scripps Research Institute. In 2003 he moved to the University of Texas Health Science Center, Houston, where he earned tenure as Associate Professor of Biomedical Informatics and Molecular Medicine. In 2007 he joined the private D. E. Shaw Research laboratory in New York City, where he participated in the historic millisecond length molecular dynamics simulation on the “Anton” special purpose supercomputer. In 2014 he returned to a academic position as Frank Batten Professor in Mechanical and Aerospace Engineering at ODU.