

MATHS AND CS WITH ICMS
2 FEBRUARY 2011
13:30-17:10
EURANDOM GREEN ROOM
(LAPLACE BUILDING 1.105)

EINDHOVEN MATHEMATICS AND COMPUTER SCIENCE
MEET THE
INSTITUTE FOR COMPLEX MOLECULAR SYSTEMS

Speakers: Bert Meijer (ST, BMT and ICMS), Tom de Greef (BMT and ICMS), Bart Markvoort (BMT and ICMS), and Kees Storm (TN and ICMS).

Intention: This is a unique opportunity for mathematicians and computer scientists at TU/e to learn about exciting research going on at the TU/e-based Institute for Complex Molecular Systems. Indeed, research that could use input from Maths and Computer Science, and the aim is to stimulate future collaboration.

Programme:

13:30-13:35: Arjeh Cohen, *Opening*

13:35-14:05: Bert Meijer, *Complex molecular systems*

14:20-14:50: Kees Storm, *Squishy Physics: Soft Mechanics of Fibrous Biomaterials*

We're interested in the stuff that we are made of. Entangled, interlinked, adaptive and dynamical arrangements of protein fibers that give tissues their mechanical properties and allow cells to move around. Physiological lengthscales are generally much, much larger than these fibers themselves - but how do we describe these materials at aggregate scales? What are the essential characteristics that must be included in multiscale models, and how do we faithfully represent the often entropic origins of mechanics at the molecular scale? I'm interested in both the a priori possibility and the feasibility of true multiscale or constitutive modeling for these materials and will tell you about some of the issues we encounter when we actually start to do so.

15:10-15:40: Tom de Greef, *Self-assembly of anisotropic interacting (macro)molecules in solution and on surfaces*

In this presentation recent efforts to understand self-assembly of anisotropic interacting (macro)molecules into fibrillar structures are discussed. The talk focuses on the mechanistic aspects that govern the transition from small to large length scales and the challenges that are encountered.

16:00-16:30: Bart Markvoort, *A model system for self-generating structures*

Amphiphilic molecules, i.e., molecules possessing both hydrophilic (water-loving) and hydrophobic (water-disliking) properties, can self-assemble into a wide variety of structures, where the structure formed is highly related to the effective shape of the molecule. One such a structure is a bilayer, which can be formed by for instance phospholipids (biological membranes) or blockcopolymers (synthetic membranes). When such membranes close on themselves they form a small container, also called vesicles. I will present some experimental and molecular dynamics simulation results showing reproduction of such vesicles and discuss some ideas and modeling questions to come to really self-reproducing systems (protocellular biomimicry).

16:30-17:00: Further informal discussion.

17:00-17:10: Closing, with view towards follow-up meetings.

Between and after the talks there will be ample time for informal discussion with the speakers in and around Eurandom's lecture rooms.