## Program

09.30 - 09.50	Registration Reception Carre Coffee in Foyer Waaier
09.50 - 10.00	Welcome by Bernard Geurts (UT-TU/e)
10.00 - 10.45	FrankNoé (FU Berlin): Conformation dynamics of biomolecules: From a variational principle to Markov models
10.45 - 11.30	Bob Planqué (VU): Mathematics for social insects
11.30 - 12.30	Posters: Flash presentations
12.30 - 13.30	Lunch and Poster session
13.30 - 14.15	Volker John (WIAS): Some recent developments in numerical methods for convection-diffusion equations
14.15 - 15.00	Ute Ebert (CWI-TU/e): Multiscale dynamics in lightning phenomena and in plasma technology
15.00 - 15.30	Coffee break
15.30 - 16.15	Alan Champneys (Bristol): Impact with friction and the Painlevé paradox
16.15 - 16.30	Closing and poster prize winning ceremony Kees Vuik (TUD)



AMI is a research center of the 3TU.Federation. It combines the strengths of the Departments of Applied Mathematics of the three Dutch Universities of Technology: Delft, Eindhoven and Twente.

Scientific Director is Kees Vuik (Delft University of Technology)

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## **Speakers**



Alan Champneys

Why is it easy to drag a piece of chalk across a blackboard, but really hard to push it? This question lies at the heart of the so-called Painleve paradox which occurs for slender bodies that can contact with a hard constaint. subject to Coulomb friction and Newtonian restitution. In this talk, which is joint work with Harry Dankowicz and Arne Nordmark, an attempt is made to formulate a general theory for planar systems. The notion of impact is complex because during energy loss, transitions can occur from stick to slip. It is argued that a so-called energetic approach due to Battle and Stronge is the most natural.

However paradoxical situations can arise during sustained contact if the coupling between lateral and rotational degrees of freedom is sufficiently large. Then the effective stiffness of the constraint surface becomes negative. We show by introducing complience and taking the infinite-stiffness limit that a unique forward simulation can be determined for all open sets of initial conditions. However, a particular degeneracy at codimension-one sets of initial conditions cannot be avoided, the presence of socalled "reverse chatter". This is the accumulation of impacts in reverse time, which leads to a fundamental nonuniqueness and is a possible explanation for the instability that occurs if you push chalk.

Mini CV: Alan Champneys got his PhD in mathematics at the University of Oxford in 1991. Following a brief postdoc at the University of Bath, he has been in the Department of Engineering Mathematics at the University of Bristol for almost 19 years, being promoted to full professor in 2001. His research interests cover nonlinear dynamics, bifurcation theory, nonlinear waves and mathematical modelling in biology and engineering. He is known for his work on homoclinic bifurcations, localised phenomena and solitary waves. More recently he has also worked on classifying dynamics that is unique to piecewise-smooth systems. Recent application domains include the biomechanics of hearing, marine renewable energy, plant morphogenisis, atomic force microscropy and autobalancers for unstable rotors.





Social insects such as ants, bees or wasps have intriqued us since the dawn of times. The sheer power they are able to muster, the dominance they can hold over other species (including sometimes ourselves!), the efficiency with which they seem to be organized, these all attest to the grandeur of social insects. In recent years there has been much work, experimental and theoretical, to understand how ant and bee colonies collectively make decisions. I will try to summarise some of this work, highlighting the role mathematics has played to gain new insights. The many levels of organization, which

are part and parcel of social insect colonies, also continue to give mathematical modellers new challenges to capture the essential features of interest. As a result, a great variety of modelling approaches is used and indeed developed, as will be illustrated in the talk.

year and a half to do a postdoc, working in the Ant Lab of Nigel Franks, before joining the VU



Convection-diffusion equations appear in the numerical simulation of many applications since they model energy or mass balances. The numerical solution even of linear convection-diffusion equations is still challenging if convection dominates diffusion, as it is generally the case in applications. In the last decades, a large amount of papers have been published which propose so-called stabilized methods. Also from the point of view of numerical analysis, many results are known, see the monograph of Roos, Stynes, and Tobiska from 2008.

This talk will present a survey and some competitive studies of stabilized methods as well as analytical results for two methods that have been obtained recently.

tific Computing at the Weierstrass Institute for Applied Analysis and Stochastics in Berlin and W3





The understanding of the most probable structures and the slow dynamics of biomolecules and other macromolecules is of fundamental importance for biochemistry and biophysics, but also has important technological applications e.g. in pharmacy and nanotechnology. The computer simulation of such molecules is limited by the famous sampling problem: the fact that the characteristic timescales of these many-particle systems are too long to be reachable by direct discrete-time-stepping simulations even when supercomputers are employed. Recently,

mathematical methods have been developed that lay the basis for divide-and-conquer such massive simulation tasks. Here we introduce the theory of conformation dynamics whose objective is to obtain the dominant eigenvalues and eigenfunctions of the transfer operator of the dynamical system. A variational principle is formulated to obtain these eigenvalues and eigenfunctions and special implementation of this variational principles, especially so-called Markov models are described. We illustrate the performance and usefulness of Markov models on a number of challenging problems, such as protein folding and allosteric changes in protein polymers.

Mini CV: Frank Noé works in the field of molecular and cellular dynamics, with emphasis on stochastic analysis and efficient simulation and analysis methods. He is known for his work in adaptive discretization in high-dimensional spaces, adapted to biophysical problems. In 2006 he defended his PhD thesis in Computer Science and Biophysics at the University of Heidelberg. After a Postdoc position in Heidelberg and a visiting professorship there as well, he was appointed Head of a Matheon junior research group at the Free University of Berlin in 2007.

> Transient discharges in ambient air are common phenomena in thunderstorms, and they are presently under development for a wide range of plasma technology, from air cleaning over energy conversion to plasma medicine. Generically the understanding of these phenomena stretches over a wide range of length and time scales. I will review present progress in hybrid modeling as well as in model reduction, including a few highlights of recent understanding.

Mini CV: Ute Ebert focuses on multiscale plasma modeling, in particular, on the dynamics of sparks and lightning. She concentrates on modeling and on the numerical and analytical aspects of calculations on multiple scales (from single electron dynamics up to the macroscopic discharge channel trees). This research is embedded in multidisciplinary projects together with applied plasma physics and power electrical engineering at TU Eindhoven and with an international network of geophysicists where she also contributes to planning and interpreting experiments and observations. She obtained her PhD at the University of Essen in 1994, and after a Postdoc position at the Lorentz institute in Leiden she joined CWI in 1998. Since 2002 she is also part-time professor at Eindhoven University of Technology.