List of Abstracts: Invited Talks

Modeling the elasto-hydrodynamics of lipid bilayers
Marino Arroyo

Lipid membranes are fundamental separation structures in animal cells, which are able to deal with conflicting requirements: they provide structural integrity and shape to multiple cell organelles and at the same time they are very malleable and constantly remodel. They accomplish this thanks to their in-plane fluidity and out-of-plane elasticity. As a result, from a physical viewpoint, membrane remodeling crucially depends on its elasto-hydrodynamics. I will discuss continuum models to understand membrane dynamics, highlighting how curvature couples the fluid and elastic responses. I will also discuss how the bilayer architecture is crucial to understand many important dynamical phenomena involving monolayer asymmetry. Finally, I will discuss the role of membrane confinement in the area regulation of synthetic and cell membranes.

Discretizing thin elastic structures
Sören Bartels

Various mathematical models in biophysics involve thin elastic structures such as surfaces or curves. The pure bending behaviour of these objects is obtained by a limit passage from three-dimensional hyperelasticity and leads to fourth order problems with inextensibility constraints. The discretization requires the use of higher order finite element methods and an appropriate treatment of the constraints. We discuss the numerical analysis and iterative solution of various effects including self-avoidance and vibrations and present simulations related to the development of microrobots for drug delivery and dynamics of microfilaments.

Willmore functional for graphs: Minimisation and gradient flow
Klaus Deckelnick

For a bounded smooth domain Ω in the plane we consider the Willmore functional for graphs subject to Dirichlet boundary conditions. The first part of the talk is concerned with the minimisation of this functional, for which we introduce and examine its L^1-lower semicontinuous envelope. Candidates for local minima of the Willmore energy can be obtained by following the Willmore flow until solutions become stationary. In the second part of the talk we therefore introduce a corresponding numerical method which uses C^1–elements. We analyse the scheme in the semidiscrete case and present results of test calculations.

Parametric finite element methods for the dynamics of fluidic membranes and vesicles
Harald Garcke

A parametric finite element approximation of a fluidic membrane, whose evolution is governed by a surface Navier–Stokes equation coupled to bulk Navier–Stokes equations, is presented. The elastic properties of the membrane are modelled with the help of curvature energies of Willmore and Helfrich type. Forces stemming from these energies act on the surface fluid, together with a forcing from the bulk fluid.
We introduce a stable parametric finite element method to solve this complex free boundary problem. Local inextensibility of the membrane is ensured by solving a tangential Navier–Stokes equations, taking surface viscosity effects of Boussinesq–Scriven type into account. In our approach the bulk and surface degrees of freedom are discretized independently, which leads to an unfitted finite element approximation of the underlying free boundary problem. Bending elastic forces resulting from an elastic membrane energy are discretized using an approximation introduced by Dziuk. The obtained numerical scheme can be shown to be stable and to have good mesh properties. We also discuss briefly how the method can be used for open membranes.
We will present three dimensional numerical computations based on the full (Navier–)Stokes system for several different scenarios. For example, the effects of the membrane viscosity, spontaneous curvature and area difference elasticity (ADE) are studied. In particular, it turns out, that even in the case of no viscosity contrast between the bulk fluids, the tank treading to tumbling transition can be obtained by increasing the membrane viscosity. In addition, we study the tank treading, tumbling and trembling behaviour for different spontaneous curvatures. We also study how features of equilibrium shapes in the ADE and spontaneous curvature models, like budding behaviour or starfish forms, behave in a shear flow.

Some simple models for vesicles and red blood cells and their implementation in a high performance computing context
Mourad Ismail

I will present some simple models for vesicles and RBCs in Fluid Flow. The main idea of this work, is to suppose that blood can be modeled by a suspension of deformable entities in a Newtonian fluid flow (plasma). These entities are subject to bending and stretching forces. The framework of the bi-fluid simulation is based on a coupling between Stokes or Navier-Stokes equations and level set method.
From the implementation point of view, we use our open source library Feel++ (`www.feelpp.org`) based on Finite Element Method and using modern (c++11/c++14) generic programming in a HPC context.

Platelet margination in tubular blood flow
Timm Krüger

I will talk about platelet margination in tubular blood flow with a special emphasis on the effects of tube diameter and the red blood cell capillary number Ca (i.e. the ratio of viscous fluid to elastic membrane forces). Platelet margination is important for blood clotting: the healing process of damaged blood vessel walls is initiated by nearby platelets. Platelets should therefore be located close to the vessel wall, ideally within the layer that is free of red blood cells (cell-free layer). The system is modelled as three-dimensional suspension of deformable red blood cells and nearly rigid platelets using a combination of the lattice-Boltzmann, immersed boundary and finite element methods. It turns out that a non-diffusive radial platelet transport facilitates margination. This non-diffusive effect is important near the edge of the cell-free layer, but only for $\mathrm{Ca} > 0.2$, when red blood cells are tank-treading. Platelets at $\mathrm{Ca} > 0.2$ eventually reach the cell-free layer where they are effectively captured. However, platelets can escape again for $\mathrm{Ca} < 0.2$. Furthermore, I will talk about the platelet dynamics once they have reached the cell-free layer.

Membranes and vesicles with bilayer asymmetry: Analytical theories and molecular simulations
Reinhard Lipowsky

Biomimetic and biological membranes consist of molecular bilayers with two leaflets that usually differ in their architecture and/or composition. Such asymmetric membranes prefer to curve in a certain manner as described by their spontaneous curvature. The asymmetry can arise, e.g., from the adsorption of small molecules [1] or from the insertion of lipids with large headgroups [2]. The associated spontaneous curvature leads to the formation of stable patterns of membrane nanotubes [3] and provides a key parameter for the engulfment of nanoparticles by membranes [4].

1 B. Rozycki and R. Lipowsky, J. Chem. Phys. 142, 054101 (2015)

2 R. Dasgupta, R. Lipowsky, and R. Dimova, Biophys. J. 108, 239A (2015)

3 Y. Liu. J. Agudo-Canaleijo, A. Grafmuller, R. Dimova and R. Lipowsky, ACS Nano (in press)

4 J. Agudo-Canaleijo and R. Lipowsky, ACS Nano 9, 3704 (2015); and Nano Letters 15, 7168 (2015)

Wrinkling dynamics of fluctuating vesicles in time-dependent viscous flow
John Lowengrub

We study the fully nonlinear dynamics of two-dimensional vesicles in a time-dependent viscous flow at finite temperature. We focus on a transient instability that can be observed when the direction of applied flow is suddenly reversed and small-scale interface perturbations known as wrinkles develop. These wrinkles are driven by regions of negative surface tension on the membrane. Using a stochastic immersed boundary method with a biophysically motivated choice of thermal fluctuations, we investigate the fully nonlinear wrinkling dynamics numerically. Different from deterministic wrinkling dynamics, thermal fluctuations lead to symmetry-breaking wrinkling patterns by exciting higher order modes. This leads to more rapid and more realistic wrinkling dynamics. Our results are in excellent agreement with the experimental data by Kantsler et al. (Kantsler et al., Phys. Rev. Lett. (2007) 99:17802). We compare the nonlinear simulation results with recent perturbation theory, modified to account for thermal fluctuations, and find that the perturbation theory misses important nonlinear interactions. While the strength of the applied flow strongly influences the most unstable wavelength characterizing the wrinkles, we find that thermal fluctuations actually have the ability to attenuate variability of the characteristic wavelength of wrinkling. This is because fluctuations excite a wider range of modes than the deterministic case, which makes the evolution less constrained and enables the most unstable wavelength to emerge.

Passive and active blood cells
Chaouqi Misbah

We will discuss modeling of blood cells (red blood cells-RBC- and leukocytes) under flow. Regarding flow of RBCs we will present three major results: (i) blood cryslas (organisation of RBC in a crystalline structure under shear flow), (ii) analogy between blood flow and traffic flow, (iii) novel partition effects of hematocrit at vascular bifurcations. Leukocyte, traditionally believed to crawl on a substratum, can swim in a very efficient way. Their swimming is qualified as amoeboid. A minimal model will be presented that captures several features of amoeboid swimming. It is found that confinement drastically affect swimming and a straight trajectory is always unstable in favor of navigation. This persistent navigation may be an indication that leukocytes have the ability of flexibly navigate through any organ without adaptations to alternating extracellular ligands, which would constitute a big constraint against an efficient immune surveillance. Finally, it will be shown that a condition of an optimal swimming reproduces the behavior of other real swimmers (like Eutreptiella gymnastica).

Recent advances in the modeling of vesicles in electric or magnetic fields
David Salac

Vesicles undergo interesting dynamics when exposed to electric or magnetic fields. Electric fields induce large deformation in the vesicle membrane and induce movement of lipid membrane domains. Alignment of vesicles in magnetic fields have also been demonstrated. Here, a recent numerical model of vesicles is presented that allows for the investigation of the electrohydrodynamics of mono- and multi-component vesicles in addition to the magnetohydrodynamics of vesicles. The model is uses an improved level set method coupled to a novel Navier-Stokes projection method which enforces local and global volume and surface area conservation. The model, sample results, and possibilities for future work will be outlined.

Computing the dynamics of biomembranes by combining conservative level set and adaptive finite element methods
Pierre Saramito

We consider the numerical simulation of the deformation of vesicle membranes under simple shear external fluid flow. A saddle-point approach is proposed for the imposition of the fluid incompressibility and the membrane inextensibility constraints, through Lagrange multipliers defined in the fluid and on the membrane respectively. Using a level set formulation, the problem is approximated by mixed finite elements combined with an automatic adaptive mesh procedure at the vicinity of the membrane boundary. Numerical experiments show that this combination of the saddle-point and adaptive mesh method enhances the robustness of the method. The effect of inertia on the stability of the vesicle in a shear flow is also investigated.

On a finite element scheme for curve shortening flow coupled to lateral diffusion
Björn Stinner

We present and analyse a semi-discrete finite element scheme for a system consisting of a geometric evolution equation for a curve and a parabolic equation on that evolving curve. More precisely, curve shortening flow with a forcing term that depends on a conserved field is coupled with a diffusion equation for that field. Such a system can be considered as a prototype for more complicated problems as they may arise in applications. In the context of biomembranes, for instance, one would expect fourth order geometric equations of elastic flow type which may be coupled to lateral reaction-diffusion equations for intra-membrane proteins. Our scheme is based on ideas of Dziuk for the curve shortening flow and Dziuk/Elliott for the parabolic equation on the moving curve. However, additional estimates particularly with respect to the time derivative of the length element are required. Numerical simulation results support the theoretical findings. Time permitting, numerical results for more complicated systems will be discussed.

List of Abstracts: Contributed Talks

Modelling and simulation of elastic cells in flow
Sebastian Aland

Accurate measurements of cell elasticity help doctors and biologists to detect diseases and physiological changes of biological cells. An innovative new technique uses a flow scenario to measure the elasticity of large amounts of cells at a rate of 100 cells per second. The idea is to flow cells through a narrow channel which leads to deformation by shear stress and pressure gradients. A comparison of the observed cell shapes with numerical simulation results permits conclusions on the elasticity of the cell.
In my talk I will address numerical methods to simulate this scenario. In particular I will present three different modeling approaches for cells flowing through a narrow channel, where cells are modeled either as (i) viscous fluids with surface tension to account for actomyosin contraction of the cytoskeleton, (ii) viscoelastic bodies to account for the viscoelasticity of intracellular components, (iii) fluid-filled elastic shells accounting for the elasticity of the cytoskeleton.
A phase field is used in all three approaches to represent the cell geometry which permits an easy mechanism to couple the cell geometry to additional equations for elasticity and surface tension. I will compare the obtained cell shapes with experimental and analytical results and draw conclusions on which the model is best-suited to describe biological cells in flow.

A finite element method for inextensible viscous membranes
Gustavo Buscaglia

A semi-implicit finite element method for the viscous inextensible flow of membranes with bending energy is presented. Surface inextensibility is addressed by either Lagrange multipliers or by penalization. Linear triangles are adopted for all unknown fields: velocity, surface pressure and vector curvature. Spurious modes are avoided with a stabilization term based on a projection of the surface pressure gradient. The penalization variant is obtained by simply increasing the dilational viscosity coefficient, which at least in our numerical experiments seems to not produce significant locking. The mesh is controled by a quality-based remeshing scheme, which is quite robust when coupled with a feedback-control of total area and volume. Numerical results are discussed in cases of relaxation, formation of tethers and thermal fluctuations.

A variational approach to particles in lipid membranes

Carsten Gräser

A variety of models for the membrane-mediated interaction of particles in lipid membranes are considered in the literature. Several of them are well established in theoretical physics but lack a rigorous mathematical analysis. We present a mathematically consistent variational framework that allows to view seemingly unrelated models as a hierarchy of successive approximations. This also allows to show new existence results for such models and makes them accessible to effective numerical methods.