Final Report

Mathematical Modelling and Analysis of Complex Fluids and Active Media in Evolving Domains

Programme held May-August 2013 at the Isaac Newton Institute for Mathematical Sciences, Cambridge, UK; organised by Uwe Thiele (Loughborough University), Darryl D. Holm (Imperial College London), Karsten Kruse (Universität des Saarlandes), Peter D. Olmsted (University of Leeds), and Len M. Pismen (Technion Haifa)

The nonlinear evolution of small amounts of complex liquids or active media bound by different types of interfaces is the subject of intense current multidisciplinary research. Mathematical models for a large variety of particular systems are derived and analysed in an intense collaboration between applied mathematics and the natural sciences. Emerging applications, e.g. in microfluidics, bio- and nanotechnology, transform the field fast into one of high importance to several engineering disciplines.

The four month programme at the INI has influenced and shaped the future research programmes and interactions of ninety scientists from the UK, Europe and overseas who discussed and further developed advanced mathematical descriptions of complex fluids and active media in adaptive domains. Thereby the programme has initiated many new collaborations between applied mathematicians and the various other communities involved in biomathematics and biophysics, soft condensed matter science, fluid dynamics, pattern formation, nano- and microfluidics, and other related fields.

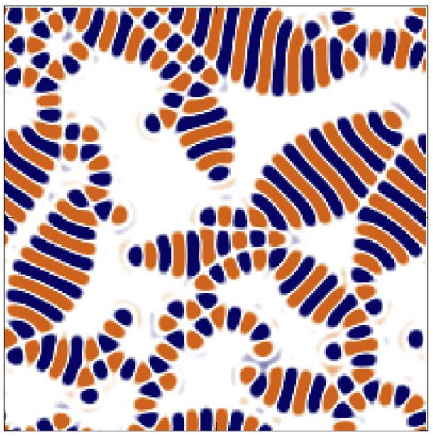

Figure 1: *Understanding soft materials: Localised states obtained through crystallisation of a binary colloidal suspension as modelled through a phase field crystal model [1].*

The study of the dynamics of complex fluids and active media in adaptive domains is an interdisciplinary quest that requires a close collaboration of researchers with very different scientific backgrounds. A joining bracket of uttermost importance are the advanced mathematical techniques that are normally developed in close interaction between applied mathematicians and the 'users' in the various other involved scientific fields. One main aim of the programme was the establishment or renewal of the communication between scientist from a spectrum spanning from geometrical mechanics - where the dissipationless motion of complex fluids is expressed combining the theory of Lie groups and differential geometry - to the physics of cell locomotion - where the dissipation-dominated motion and development of the cytoskeleton is expressed through models for active fluids. The aspect of the adaptive domains furthermore incorporated the discussion of the many problems related to the motion of various types of two-phase interfaces and three-phase contact lines.

Topics and problems that led to many discussions of open problems and, in consequence, initiated new collaborations include

- Geometric mechanics descriptions of complex fluids as, e.g., micropolar liquids, the Euler-Poincaré approach; incorporation of dissipation and interfaces into this framework.
- Gradient dynamics descriptions for interface- and dissipation-dominated layers of complex fluids.
- Microscale molecular dynamics simulations of complex fluids, e.g., drops on solid substrates or membranes their relation to microscale and mesoscale continuum models, as dynamical density functional theory (see Figure 1) and hydrodynamic gradient dynamics models, respectively.
- Mathematics of coarse-graining and upscaling techniques in the context of complex fluids, cross-

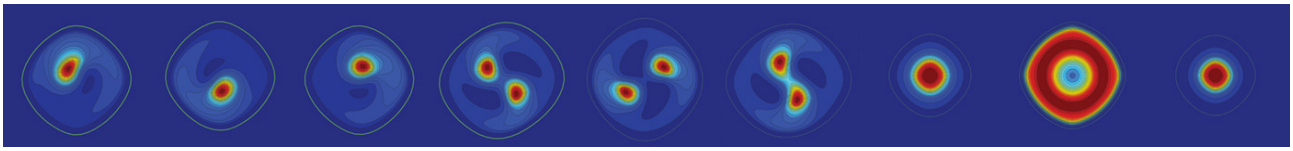

Figure 2: *Understanding cell motility: Snapshots of spontaneous actin waves in domains with dynamic boundaries modelled through a mesoscopic description of treadmilling actin filaments. One- and two-armed spirals and a breather. Warm colours represent high, cold colours low actin densities [2].*

usage of techniques, e.g., coarse bifurcation analysis for microscopic simulators.

- Nonlocal evolution equations, their well-posedness and analysis.
- Mechanics of living cells, which involves complex problems of modelling an active medium with rheology combining viscoelasticity, anisotropy, and multiphase features, coupled to chemical transformations, diffusion, and active transport (see Figure 2).
- Mathematical description of the motion of single crawling and swimming cells, bacteria and artificial microswimmers; collective dynamics of microswimmers, dynamics and growth of biological membranes, biofilms and tissues.
- Relation of equilibrium and non-equilibrium behaviour of complex and active fluids, relation of the decription of active media to classical kinetic equations.
- Asymptotic and numerical methods for kinetic equations describing complex fluids, role and description of defects, topological phases.
- Interaction of complex fluids with boundaries.
- Interface dynamics for complex fluids, the coupling of internal degrees of freedom and interface motion, e.g., for liquid crystals, nanoparticle suspensions and polymer solutions; drying and crystallisation fronts, patterned deposition from moving fronts
- Shear-induced transitions in complex fluids, shear-banding, micro-structural rearrangement. Control through boundary conditions.

The list illustrates well that complex fluids in the combination with interfaces are a challenge not only with respect to the development of mathematically and thermodynamically consistent models but also with respect to the subsequent analysis of system behaviour that is often marked by the interplay of different instabilities that trigger hierarchical structure formation processes, developing singularities and the dynamics of emerging defects. Addressing such problems, the programme at the INI has resulted in a further cross-fertilisation between fluid mechanics and mathematical theory, driving both the development of perturbation methods and other analytical tools, and the understanding of related physical phenomena.

The described wide scope of the programme presented a challenge that was successfully tackled through a combination of many seminars, crash courses, informal discussion meetings, workshops and many individual discussions that involved all the participants from world leading experts to junior faculty, postdocs and phd candidates. During the first two months the programme enjoyed the multifaceted interaction with the parallel INI Programme *The Mathematics of Liquid Crystals* organised by John Ball and colleagues. The partial overlap resulted in many cross-programme activities from common seminars and discussions, shared participants, exchange of seminar speakers and two workshops (*Dynamics of active suspensions, gels, cells and tissues* and *Liquid Crystal Defects and their Geometry, Active and Solid Liquid Crystals*) that were held in parallel with shared sessions on subjects of common interest, in particular, related to active soft matter. The interaction was very fruitful for both communities and increased the outreach of both programmes. The Rothschild Visiting Professor for the programme was Peter Constantin (Princeton University), and the Microsoft Research Visiting Fellow was Yannis Kevrekidis (Princeton University).

Beside the continuous seminar programme with the programme fellows and participants, the wider community, in particular, including more young scientists were involved through the two embedded workshops and the extended summer school. One of the workshops was held at the University of Leeds reaching out to the scientific community of Northern England. Furthermore, the embedded summer school on *Multiscale and hybrid methods for complex fluids* attracted many young promising researchers. Here, the combination of a two-week duration with lectures on a wide variety of different approaches to complex fluids and active media proved to be a very attractive format. The combination of short contributions and longer instructional courses particularly allowed younger researchers to better integrate concepts of mathematical modelling and non-equilibrium, nonlinear, and soft matter science into the presently active research fields. Most of the younger participants also obtained feedback on their own research as their posters were on display throughout the school allowing for discussions with the leading experts not only during the two evening poster sessions.

As a result of the programme we have seen the emergence of new collaborations, the development of new research projects that will shape the field in the near and far future. Most of the lectures and seminars throughout the programme were streamed through the internet, and were watched by colleagues worldwide, that were not able to attend the INI in person. The resulting video archive will prove to be a very valuable source of knowledge and inspiration that will ensure the continuing influence of the Programme. To conclude, we believe that the programme has been instrumental in overcoming the developing fragmentation of the field and in this way has opened opportunities to trigger major future advances.

References

[1] M. J. Robbins, A. J. Archer, U. Thiele, and Knobloch E. Modelling fluids and crystals using a two-component modified phase field crystal model. *Phys. Rev. E*, 85:061408, 2012. **doi:**10.1103/PhysRevE.85.061408.

[2] K Doubrovinski and K Kruse. Cell motility resulting from spontaneous polymerization waves. *Phys. Rev. Lett.*, 107:258103, 2011. **doi:**10.1103/PhysRevLett.107.258103.