Long report: *The Mathematics of Multiphase Flows with Applications* (INI Satellite Meeting)

Dates: 2nd July - 26th July 2024

Venue: University of East Anglia

Organisers: Prof. Mark Blyth, Prof. Alexander Korobkin (UEA, Mathematics), and Prof. José Manuel Gordillo (University of Seville, Spain)

1. Context

A multiphase flow occurs when different phases/components (gas, liquid and solid) coexist and interact dynamically. Complex flows of this nature pose many mathematical challenges, but understanding them is vital given their relevance to natural processes and industrial applications. Examples of multiphase flows include viscosity and density stratified flows, flows with phase changes (e.g. melting, evaporation), aerated and bubbly flows, suspensions and colloids, hydroelasticity, and flows involving capsules, particles and cells. Natural science applications include disease transmission (e.g. for airborne respiratory infections such as COVID-19), coating flows including clinical applications of 3D printing for artificial limbs, blood flow in the cardiovascular system, biofilms, cavitation bubbles in plants and trees, volcanic flows and soil erosion. Industrial and engineering applications include the transportation of Liquid Natural Gas (LNG) [R1], aircraft wing icing, renewable energy generation, heat and mass transfer devices, wave impacts on floating structures, and chemical reactions and combustion.

The central theme of the programme concerned the reliable mathematical modelling of multiphase flows. Even with the substantial computational power that is available nowadays, modelling and computing these types of flows remains a major technical challenge. In some problems, multiphase systems can be considered as complex homogeneous fluids with specific equations of state and specific thermodynamic properties. In other problems, each phase should be traced separately, properly accounting for interactions between phases and phase changes including the interfaces and free boundaries. Often the flows are coupled and highly nonlinear. From a mathematical perspective, meeting the challenge posed by such complex systems requires sophisticated use of modelling techniques, analytical approaches including asymptotic analysis and stability analysis, and Direct Numerical Simulations (DNS). Modern DNS approaches, including both continuum approaches (e.g. volume-of-fluid methods) and discrete approaches (e.g. molecular dynamics and Lattice-Boltzmann approaches) are powerful and can provide intricate detail across a range of scales, yet they remain computationally expensive particularly when applied to more complex phenomena (e.g. topological transitions such as jet break-up or dripping). Physical insight and understanding requires parsimonious models that operate with a limited number of parameters to supply a reasonable level of explanation and predictive capability within a tractable mathematical framework. Mathematical advancement comes from a unified approach that combines the detailed numerical data available from DNS with the physical gains afforded by simplified models, all channeled through a properly constructed feedback loop to be validated and verified at every step.

2. Outline and goals of the programme

In this month-long programme our aim was to showcase the state-of-the-art in multiphase flow research, and to bring together experts and early career researchers to work in a stimulating, interdisciplinary and research intensive environment that would foster collaboration, provoke new ideas, and instigate new advances. The emphasis was on the mathematical challenges posed by multiphase flows with interfaces and free boundaries. However, recognising that a fully comprehensive approach must combine theoretical perspectives with physical insight and practical experience, we also sought participation from engineers and experimentalists.

The programme took place at the University of East Anglia (UEA) from 2nd to 26th July 2024. In keeping with our aim to shine a spotlight on the excellent multiphase flows research that takes place at UEA, we included participants from various schools and partners across the Norwich Research Park. This included participants from the UEA School of Environmental Sciences, the School of Biological Sciences, the School of Engineering, and from the John Innes Centre, which specialises in the plant science. These participants gave less technical presentations intended to highlight the multiphase flow phenomena and problems arising in their own fields. These included presentations on volcanoes and volcanic eruptions, the biomechanics and human and animal sperm, lithium battery design, wetting phenomena on complex geometries, and liquid-liquid phase separation in plant phloem. Overall, the assembled list of programme participants covered a wide range of mathematical expertise including analytical techniques (e.g. asymptotics), stability theory, boundary layer theory, numerical computation and DNS, methods for control, and phase field methods.

The working environment for the programme was carefully considered to allow for an atmosphere to stimulate knowledge exchange, discussion and collaboration. The programme timetable was as follows:

Week 1: Early Career Researcher (ECR) Summer School

Week 2: Programme workshop *New Directions in Multiphase Flows*, including an ECR poster session.

Weeks 3 & 4: In-residence research programme.

The programme also included a public lecture that was held in the Thomas Paine Study Centre, delivered by Dr Javier Rodríguez Rodríguez, and entitled ‘From beer tapping to volcanic eruptions and supernovae: the physics of mass transfer’. The public lecture was slotted to run immediately after the ECR poster session to give the public a chance to sample a range of research taking place across the programme. A drinks reception was laid on after the public lecture to encourage attendees to stay afterwards to view the posters and chat with the poster presenters.

3. Specific Events

Early Career Researcher (ECR) Summer School

The Summer School attracted 36 participants. It provided Early Career Researchers with a broad training in mathematical techniques for multiphase flows, including both theoretical and numerical approaches. The week was broken down into morning and afternoon sessions dedicated to particular topics. The lecturers were Dr Susana Gomes and Oscar Holroyd (University of Warwick), Professor James Sprittles (University of Warwick), Professor Demetrios Papageorgiou (Imperial College, London), Professor Darren Crowdy (Imperial College, London), Dr Mirco Magnini (University of Nottingham), and Dr Radu Cimpeanu (University of Warwick). The specific sessions were as follows (abstracts are included in the Appendix):

Dr Susana Gomes and Oscar Holroyd (University of Warwick): *Introduction to control and some applications to interfacial flows*

Professor James Sprittles (University of Warwick): *Multiphase Flows at Small Scales: Beyond Navier-Stokes*

Professor Demetrios Papageorgiou (Imperial College, London): *Using asymptotics to probe the nonlinear dynamics of multilayer flows*

Professor Darren Crowdy (Imperial College, London): *Analytical methods for multiphase flows*

Professor Dr Mirco Magnini (University of Nottingham): *Interface-resolved Simulations of Multiphase and Evaporating Flows with OpenFOAM*

Professor Dr Radu Cimpeanu (University of Warwick): *At the interface between analytical approaches and high performance computing in fluid mechanics*

In addition to the scientific elements of the summer school, several social events were organised, including a pizza and drinks event, and a ten-pin bowling and food evening at a local bowling house in Norwich.

Programme Workshop: New Directions in Multiphase Flows

The centrepiece of the programme was the programme workshop, which was held in the second week from 8th to 12th July. Each of the five days of the workshop started with a plenary lecture followed by sessions of invited talks covering a wide range of topics in multiphase flows research. The plenary lecturers were:

- Andrew Hazel (University of Manchester, UK)
- Stéphane Zaleski (Sorbonne University, France)
- Stephan Gekle (University of Bayreuth, Germany)
- Christophe Josserand (CNRS & LadHyX, École Polytechnique, France)
- Claus-Dieter Ohl (Otto-von-Guericke University, Germany)

The workshop attracted 72 participants. Aside from mathematicians, participants at the workshop represented a range of backgrounds including engineering, physics, plant science, and included theoreticians as well as experimentalists. Industry was represented by AeroTex UK and Bureau Veritas, France. Industrial presentations covered aircraft icing and phase change effects during Liquid Natural Gas sloshing. The workshop presentations covered many aspects of multiphase flows research including bubble dynamics, evaporation of liquid drops, biological tissue growth, blood flow, cavitational collapse, moving contact lines, foams, liquid films, control methods, fluid-structure interaction, computational methods including deep learning methods, sloshing, boiling, droplet impact, ice particles in flow, gels, thermal management for batteries, surfactants, and flexural gravity waves. In total there were 33 presentations. A poster session for Early Career Researchers was held on 11th July, which included 19 posters covering various multiphase flows problems. An informal discussion session on 'Liquid Impact' was led by A. Korobkin during the lunch break on the 11th of July. The meeting was recorded with 18 participants in attendance.

In addition to the scientific components of the workshop, several social events were organised, including a drinks reception and a workshop dinner held in the Sainsbury Centre for the Visual Arts on the UEA campus.

In-residence programme

The final two weeks of the programme comprised the in-residence programme. This included up to 27 participants. Open plan office space was provided to participants including two main rooms and a side room that could be used for Zoom/Teams meetings. The two main rooms included the 'noisy room', intended for formal presentations as well as open discussion, and the 'quiet room' which was intended to provide a quiet space for working without distraction. The quiet room was set up with a snack stall and a coffee machine for the use of participants.

The in-residence programme included formal research seminars given by the programme participants and by various invited speakers including those working at UEA and on the wider Norwich

Research Park. Most days included a single seminar, but on two of the days two seminars were presented. The speakers and talk titles were as follows:

• Jack Panter (University of East Anglia) *Wetting on complex geometries: from organisms to algorithms.*

• Jorge Arrieta Sanagustin (University of the Balearic Islands) *On the flow separation mechanism in the inverse Leidenfrost regime*

• Jess Johnson (University of East Anglia) *Multi-phase fluids in and around Volcanoes: Challenges and current state-of-the-art*

• Alice Thompson (University of Manchester) *Feedback control and control-based continuation for deformable bubbles*

• Javier Rodríguez Rodríguez (Carlos III University of Madrid) *Evaporation dynamics of respiratory-like droplets and their implications on virus infectivity*

• Nikos Pelekasis University of Thessaly *Computational fluid dynamics and stability of interfacial phenomena in the presence of acoustic, viscoelastic, adhesive, and Lorentz forces*

• Simone Immler (University of East Anglia) *The role of micro-fluidics in sperm performance and fertilisation*

• Peter Hicks (University of Aberdeen) *Liquid-solid collisions with pre- and post-impact gas cushioning*

• Richard Morris (John Innes Centre, Norwich) *Predictive modelling of phase-separation: computer-guided engineering of protein condensation*

• Doireann O'Kiely (University of Limerick) *Floating elastic and viscous sheets: fluid-solid and fluid-fluid interactions during wrinkling and buckling*

In addition to these, an informal discussion session, led by Prof. Nikos Pelekasis (University of Thessaly) was held on the morning of Wednesday 24th July covering *Spreading of a liquid metal coating in the presence of adhesion and Lorentz forces.*

In addition to the scientific elements of the in-residence programme, several social events were organised. These included a trip to the National Trust property Blickling Hall in Aylsham, a BBQ, and an end-of-programme meal at a local restaurant.

4. Scientific Outcomes and Highlights

The study of multiphase flow phenomena presents significant challenges to the scientific community. A key difficulty faced by the multiphase flows researcher concerns the tracking of the interface, or interfaces, between phases, and the possibly highly complex multiphysical effects and processes that may be taking place at these interfaces. Physical effects include, for example, surface tension, Marangoni tractions (driven, for example, by the presence of surfactants or via thermocapillary effects), and electric and magnetic forces. Phase change may occur a the boundary between interfaces, for example via evaporation or solidification. Suitable transport and/or reaction equations may be required to properly account for the interfacial physics (e.g. to account for the interfacial convection and/or diffusion of surfactant molecules). The presence of moving contact lines also presents a theoretical challenge.

An important outcome from the meeting was the strong recognition among participants that addressing these challenges requires collaboration between scientists with different expertise, including theoretical analysis (e.g. asymptotic analysis), modelling and physics, full-scale numerical computation, and experimentation. The range of talks and discussions during the programme covered the spectrum of these approaches, introducing participants to new ideas and new concepts, and new approaches to tackling problems. Notable examples of cutting-edge methods discussed at the programme included deep learning techniques for solving PDEs, novel methods for interfacial control, and DNS simulations via Basilisk and OpenFoam. A notable highlight was the realisation, from experimental observations, that damage caused by near-wall bubble collapse is not associated with jet formation, as many had hitherto understood, but via the effect of shock wave self-focusing.

Collaborations

Several potential new collaborations on new projects were established at the meeting. In other cases existing collaborations were helped to continue. These include:

- C. Josserand, J. Rodríguez-Rodríguez, J. Arrieta & A. Korobkin: Assembling/aggregation of bodies floating on a thin liquid layer.
- M.-J. Thoroval, A. Korobkin: Impact of droplets with rigid/bubble inclusions.
- R. Cimpeanu, M. Moore, C. Josserand & A. Korobkin: Impact of two different fluids.
- J. Arrieta & M. Blyth: Flow separation in the inverse Leidendrost regime.
- R. Cimpeanu, D. Tseluiko, T-S. Lin & M. Blyth: Dynamics of an inverted liquid film.
- M. Afzaal & M. Blyth: Modelling high-speed liquid jets.
- Y. Semenov & M. Blyth: Detachment streamlines with surface tension
- J. Arrieta & J. Rodriguez-Rodriguez: Aggregation of proteins at interfaces.
- F. T. Smith, J. Jepson & M. Iccardi: Moving phase-change interfaces
- F. T. Smith & J. Jepson: Melting and freezing of in-flow ice particles.
- J. Rodríguez-Rodríguez, M. Moore & A. Wray: Formation of aggregate particles in evaporating drops
- J. Rodríguez-Rodríguez & J. Sánchez: Interaction of floating objects
- J. Rodríguez-Rodríguez & J. Ruiz Rus & Carlos Martinez Bazán: Modelling of the coalescence of a cloud of bubbles.
- A. Askounis, M. Moore & A. Wray: Droplets
- L. Biancofiore & Doireann O'Kiely: Homogenisation of rough channels lubricated by viscoelastic films.
- L. Biancofiore & M. Magnini: Bretherton bubble in a Couette flow and DNS of an evaporating thin film.
- A. Kalogirou, E. Green, A. Tam: discussions to propose a Nottingham-Adelaide joint PhD project.
- A. Kalogirou, A. Hazel & M. Blyth: multilayer channel flow with surfactants.
- A. Hazel & D. Netherwood: Simulations of flow in collapsible tubes and of biological transport.

Appendix. ECR Summer School - class abstracts

Dr Susana Gomes and Oscar Holroyd (University of Warwick): *Introduction to control and some applications to interfacial flows*

Abstract: Falling liquid films are typical interfacial flows which exhibit an interesting range of

behaviours, from flat films to travelling waves and chaotic-looking interfaces. They are a canonical problem in fluid dynamics and have a range of industrial applications, including coatings or microchip cooling. In these applications, we would therefore want to control them to have a desired interface shape. I will introduce some results in control theory (from linear control theory applicable to ODEs to nonlinear optimal control problems) and show how to adapt these to be applied to nonlinear PDE models for the interface of these films. We'll discuss robustness of controls across models, and finally show how they perform in direct numerical simulations of the Navier—Stokes equations for the full problem.

Professor James Sprittles (University of Warwick): *Multiphase Flows at Small Scales: Beyond Navier-Stokes*

ABSTRACT: The conventional Navier-Stokes modelling paradigm gives remarkably accurate results for a wide range of fluid flow phenomena. However, when layers of fluid become sufficiently thin, additional physics, conventionally neglected, becomes prominent. In this talk, I will introduce some of this additional physics and explain how it can be incorporated into a computational modelling framework that 'goes beyond' the traditional Navier-Stokes setup. Specifically, gas kinetic effects, disjoining pressure and thermal fluctuations will be shown to have a dominant effect on a number of commonly observed and technologically-relevant flows, such as the collision dynamics of liquid droplets and the stability of thin liquid films.

Professor Demetrios Papageorgiou (Imperial College, London): *Using asymptotics to probe the nonlinear dynamics of multilayer flows*

ABSTRACT: Immiscible multilayer flows are challenging due to nonlinearities in both the governing equations (Navier-Stokes systems) and the free surfaces/interfaces that must be determined as part of the solution. Nonlinear deflections can lead to singular effects such as dewetting and topological transitions. This set of lectures will explore, from first principles, the powerful use of multiscale asymptotic analysis in deriving physically relevant reduced order models. The models will be analysed and computed with emphasis placed on the supported intricate nonlinear phenomena that would be extremely hard to access using direct numerical simulations. Multiphysics effects such as external electric and magnetic fields, surfactants are also amenable to analysis and key elements will be presented.

Professor Darren Crowdy (Imperial College, London): *Analytical methods for multiphase flows*

ABSTRACT: Compared to single-phase flows, analytical methods for multiphase flows interacting across an interface are rare, even in two-dimensional model problems where many tools (e.g. conformal mapping) that are useful in single-phase problems fail. These summer school lectures will survey some of the analytical methods for multiphase flows that do exist, including novel numerical schemes based on them, with special focus on recent examples pertaining to problems of current interest in modern multiphysics applications. The aim of the lectures is to spur interest in developing new mathematical tools and approaches for modelling multiphase flows.

Professor Dr Mirco Magnini (University of Nottingham): *Interface-resolved Simulations of Multiphase and Evaporating Flows with OpenFOAM*

ABSTRACT: This session will provide an introduction to the most established techniques for the direct numerical simulation of two-phase flows, with a specific focus on the Volume Of Fluid method and on the opensource simulation toolbox OpenFOAM. The session will cover the key ingredients for accurate interface-resolved simulations, from interface advection, to surface tension and phase-change. Hands-on sessions will provide an opportunity for participants to practice benchmark flow configurations using OpenFOAM and a custom solver for flows with phase change, installed in a self-contained virtual machine running a linux operating system.

Professor Dr Radu Cimpeanu (University of Warwick): *At the interface between analytical approaches and high performance computing in fluid mechanics*

Abstract: During this session we will explore how analytical techniques can work hand in hand with accurate numerical methods in order to enhance both the range of validity and efficiency of each strategy. Rather than disparate individual approaches, we will instead try to position ourselves at the centre of large scale evolving communities, building an interdisciplinary skillset along the way. We will (perhaps unsurprisingly) tackle interfacial flow problems that enable both meaningful analytical progress via modelling and asymptotic techniques, and hands-on numerical work using the volume-of-fluid method. The session will be highly interactive, with framework code provided and group work encouraged. We will spend ample time also discussing elements of good practice in this space, from version control to how to build, maintain and disseminate sustainable software for the applied mathematical community. No prior experience required, but a setup with (and working knowledge of) a UNIX-based operating system could be quite useful - if not already in place, this will be a good opportunity to meet new colleagues as part of the group discussions and practical elements of the session.