Research Statement

Motivation

The rhythmic beating of cilia attached to motile organisms, the crashing of ocean waves onto offshore oil platforms and the spray cooling of steel sheets in industry are all examples of the simultaneous interaction of multiple physical forces over several length and timescales. Such multi-physics and multi-scale problems are notoriously difficult to study both experimentally and from a modelling perspective. One difficulty in the mathematical modelling of such problems is the ubiquitous presence of distinct, moving and interacting, fluid-fluid or fluid-solid interfaces within a single physical system. My own research interests lie in the computational modelling of such multi-phase problems, both in engineering and the natural sciences. My research motivation is the further understanding of such physical processes through the development of model methodology and the application of new and innovative solution methods.

Research History

A Industrial/Engineering Research

After completion of an undergraduate degree in applied mathematics I became involved in industrial and engineering research (listed in chronological order):

- As a vacation scholar (1992-1995) at BHP Melbourne Research Laboratories in Melbourne, Australia investigating the non-contact temperature measurement of steel sheets in industry through infra-red pyrometry and microwave radiometry. This required an accurate knowledge of the surface emissivity of hot steel sheets covered in several layers of iron oxide. Interest in this field was the precursor of the work done in my Masters Thesis entitled "A Theroretical Investigation of Steel Surface Emissivity"; which led to several papers concerning the emissivity of rough oxidised steel surfaces and were presented in two Asia Pacific Microwave Conferences.
- As Research Consultant (2000-2001) in the Department of Mechanical Engineering at the University of Wollongong, Wollongong, Australia, in collaboration with Professor Wee-King Soh involving the water-jet cooling of hot steel sheets in industry through the solution of a temperature transport equation using an Eulerian-Lagrangian (EL) method. This work also led to papers in the *Journal of the Australian Mathematical Society* and a conference paper at the *International Symposium in Computational Heat Transfer* as well as invitations to other heat transfer conferences.
- As Research Scientist (2001-2004) and member of the research team led by Dr Paul Zulli at BlueScope Steel Research Laboratories, Port Kembla, Australia, studying the influence of a taphole clay pedestal on fluid flow and heat transfer within a blast furnace as well as the significance of the coke-free layer on fluid flow and heat transfer in a blast furnace. This work involved the modification of commercial CFX-4 software for the numerical modelling of heat transfer and fluid dynamics in a porous medium.
- As Associate Research Fellow (2005) in the School of Mathematics and Applied Statistics at the University of Wollongong, Australia, collaborating with Dr Mark Nelson to work on the pharmaceutical application of drug release from swelling hydrogels. Drugs are placed inside biocompatible hydrogel polymers which, upon immersion into the body, release the drug gradually maintaining the optimal concentration in the bloodstream. The research problem investigated how the swelling of the hydrogel, as it absorbs water from its surroundings, effects drug release.
- As Research Associate (2006-2009) in the School of Mathematics at Cardiff University under the supervision of Professor Tim Phillips developing multiphase flow models for droplet dynamics involving complex flows (EPSRC grant EP/C513037) using an Eulerian-Lagrangian method as well as developing Lagrangian particle methods for viscoelastic flows using Smoothed Particle Hydrodynamics. This work led to several papers including one in the *International Journal for Numerical Methods in Fluids* as well as the *ILASS'08* conference.
- As Research Fellow (2010-2011) in the School of Mechanical Engineering at the University of Leeds linked to industry via a collaborative research grant from the Technology Strategy Board and GlaxoSmithKline. The project's purpose was to optimise a novel technology where active pharmaceutical ingredients are printed onto a carrier tablet in a process akin to inkjet printing. This involved the CFD simulation of the drop formation process: where fluid is forced through a capillary nozzle, causing it to form a pendant hanging droplet which first pinches off from the

nozzle and then impacts onto the surface. The project studied how this process takes place with regard to the fluids used and the operating conditions involved.

- As Lecturer (2012-2013) in the School of Computing, Mathematics & Digital Technology at Manchester Metropolitan University I carried out research work in various areas including: (i) analytical solutions to determine the emissivity of rough steel surfaces in the steel industry (upcoming *BAMC 2013*), (ii) a new algorithm to resolve the presence of artificial numerical pressure boundary conditions in incompressible projection methods (upcoming *BAMC 2013*) and (iii) the effect of capillary waves in the ejection process of pendant drops.

B PhD Thesis Work

The connection to industrially applied research continued during my PhD involving the development of optimal numerical modelling methods for the impact of water droplets onto hot galvanised steel surfaces. The solidification of the molten zinc layer (galvanisation) on top of the sheet while being impinged by water droplets within a spray gave rise to a cratered or roughened surface which best binds to other materials such as concrete. The thesis concentrated on the difficult problem of three phase flow, areas of specific concern were how best to:

a) impose boundary conditions at a fluid-fluid interface and track it accurately while it undergoes severe deformation and disruption
b) maintain and impose incompressibility within each fluid as well as the boundaries over the whole solution time
c) model fluid advection and viscosity in the presence of high density ratio fluid-fluid interfaces

Research Contributions

The solution of this problem was formulated within a one-field model using an Eulerian-Lagrangian mesh-particle discretisation of immersed fluid-fluid interfaces avoiding the need to separately impose interfacial boundary conditions and taking advantage of each of these techniques. This is categorised in terms of interface tracking and as a general multiphase flow solver:

(i) <u>Lagrangian Interface Tracking</u>*:* this research possesses some unique advantages over other previously developed interface tracking methods:

- Particles were assigned to track only fluid phase information this avoids the various instabilities which persist in pure particle methods but possesses several advantages.
- Fluid colour is assigned permanently to each fluid so that fluid identity is maintained throughout the flow.
- Colour information is interpolated to the underlying grid in only one direction avoiding artificial numerical diffusion of fluid interfaces.
- Fluid identity is conserved at smaller than grid resolution thereby avoiding artificial numerical surface tension which results in the non-physical clumping of fluid blobs.
- The method is of second order accuracy while maintaining a constant interfacial transition width no matter the severity of interface disruption. These results were published in *Computers & Fluids*.

(ii) <u>Eulerian Multiphase Flow Solver</u>*:* The interface tracking method I developed in the previous paper was combined with an approximate projection method to ensure incompressibility up to second order while avoiding grid decoupling in the pressure and velocity. The Godunov method was used to accurately advect fluid velocities without inducing instabilities during rapid changes of material properties across fluid interfaces. Pressure correction is implemented within the variable density solver so that artificial numerical boundary layers are not present. The method showed promising behaviour when measured against the experimentally determined radial spread factor for the droplet-solid impact and cavity depth for the droplet-liquid impact problem.

Current Research

Research Contributions

A Multiphase Flows & Droplets

Research during the Cardiff postdoc expanded the previously developed multiphase flow code to take into account surface forces and the inclusion of outflow conditions to allow truncation of the computational domain. The new code has been applied to:

(i) Droplet Break-Up: This problem is commonly encountered in diesel engine fuel sprays and in spray cooling or painting. Experimental observations demonstrate different break-up modes depending on critical Weber number including: vibrational, bag, sheet stripping and catastrophic break-up. The

method was able to accurately model both vibrational and sheet stripping behaviour although the bag break-up process requires higher resolutions as this instability occurs at length scales below the resolution used. (published in *International Journal for Numerical Methods in Fluids*)
(ii) Multi-Droplet Interaction in Spray Impingement: It is often claimed that the characteristic impact behaviour of an individual spray droplet may be extrapolated to multiple droplets within the spray. However, upon the simulation of up to three impacting droplets this is found to be very different. Provided the impacting droplets are within the influence zone of each other the droplets will interact significantly. (published in proceedings of *ILASS 08*)
(iii) The Role of Neighbouring Droplets in the Spray Break-Up Process: The surface to volume ratio of fuel droplets within a diesel engine determines combustion efficiency so that an understanding of spray break-up is vital to this process. How nearby droplets in the spray influence this process is not well understood. The numerical simulation of the break-up behaviour of two equally sized droplets in two distinct geometrical configurations shows that the break up of each droplet is strongly influenced by the presence of the other. (published in proceedings of *ILASS 08*)

B The Drop Formation Process
My more recent research at the University of Leeds modified an existing Lagrangian finite element code, originally designed to simulate the inkjet process, in order to model the drop formation process which occurs at the larger length and time scales required for the pill printing process:

Operability Windows in the Industrial Drop Formation Process: GlaxoSmithKline has developed a way of printing active pharmaceutical ingredients onto tablets. Printing onto pre-formed tablets speeds up and improves quality control, as each tablet contains exactly the correct dose as well as being faster acting. This study developed a computational tool to accurately predict the behaviour of the printing process, subject to the operating conditions of the plant equipment and the properties of the fluid itself. These operability diagrams are an important tool for use in the industrial process. (*paper to be published in upcoming AMIS 2012 Conference Proceedings*)

C Mesh-free Methods
The Treatment of Boundary Conditions in SPH: The particle deficiency problem in the presence of a rigid wall in Smoothed Particle Hydrodynamics arises from insufficient information being available to perform accurate interpolation of data for particles located nearer to the boundary than the support of the interpolation kernel. I developed a consistent treatment of no-slip boundary conditions to obtain approximations to the velocity of image particles. The method is validated for Poiseuille and Couette flow, for which analytical series solutions exist**.** (published in *Computer Methods in Applied Mechanics and Engineering*)

Research Agenda

My experience in engineering and industrial research has shown me the importance of two aspects in the modelling process. Firstly, in model methodology: the development of new mathematical models and the construction of innovative numerical methods and secondly: the application of these newly developed models/methods in the solution of complex natural, engineering and industrial problems.

Research Directions

A Model Methodology

Physical modelling & numerical compatibility: typically such mathematical models involve the modelling of complex physical systems and the solution of the associated partial differential equations for reasons (i) involving the interaction of continuous (Eulerian) and discrete (Lagrangian) media, e.g. soil erosion through water-drop impact, and (ii) of numerical compatibility, e.g. the interaction of multiphase flows in an Eulerian medium involving the solution of multiple material advection equations for which a Lagrangian description is ideal.
One-Field Models, Variational Principles & Optimised EL Systems*:* a fuller development of the one-field approach as a general tool for multi-physics problems which allows the interaction of multiple physical forces within a single framework incorporating multiple materials: solid, elastic, fluid while still allowing interfacial immersed boundary conditions to be satisfied in a natural way. This involves the process whereby a continuous EL model is created so that many of the internal aspects of the

model, such as immersed forces, may be constructed. A similar process is proposed in order to optimise a numerical discretisation of the original continuous EL system so that error growth is minimised.

B Applications

1. Biological Flows: for example: the wind dispersal of seeds is a function of the presence of wind to lift the seeds and the structures used by the seeds to remain aloft. These kinds of structures, immersed within an ambient fluid, may be examined in order to determine the maximum dispersal of seed. Other examples of biological flows include cell motility in bacterial chemotaxis, as well as filter and suspension feeding.
2. Soil Erosion: the application of multi-physics, multi-phase one-field methods to the mathematical modelling of the poorly understood raindrop induced splash erosion (rainsplash) process. This involves a model able to capture all of the significant features of the process such as cratering, splashing and flow transport of loosened soil particles within a water-soil suspension flow

Research Initiatives

A Short Term Goals (1-3 years)

My main aim in the short term lies in two directions. Firstly, the development of innovative new techniques to codes I have already developed for incompressible multiphase flows as described in the "Research History" and "Current Research" sections above. Secondly, the development of truly optimised One-Field, Eulerian-Lagrangian codes so that each is best utilised within the overall goal of fast, accurate and robust solution techniques for incompressible multiphase flow.

1. New Developments*:* there remain several outstanding issues in incompressible multiphase flows including:
(i) Projections methods: to further develop numerical methods to more accurately solve the discontinuous Poisson equation arising within the one-field setting as well as satisfying incompressibility to at least second order while avoiding the creation of numerical boundary layers on no-slip walls.
(ii) Mesh-Particle Methods: to formulate a better understanding of how fixed Eulerian grids and Lagrangian particles interact in multiphase flow problems.
(iii) Immersed Forces: to develop new multi-material force models in order to: (i) eliminate or minimise parasitic currents in multi-fluid models, (ii) model and incorporate immersed materials and boundaries at multiple length scales.

2. Optimised Methods: the issues raised above are important but they do not study how these individual methods combine together in an optimal way to best model the physical systems in question. This approach must focus on: (i) the physical forces acting, (ii) the materials involved: solid, fluid elastic, (iii) the underlying length and timescales and (iv) the geometry of the problem.

B Mid Term Goals (3-5 years)

The development compressible multiphase flow codes to take into account fluid density changes encountered in solidification, evaporation, boiling and highly compressive dynamics such as sound waves or explosions.

C Long Term Goals (5+ years)

(i) Commercial Applications: Upon sufficient development of the previous research into fast, accurate, robust codes of high fidelity I aim to implement the code either within existing commercial software, e.g. CFX, or in-house software designed specifically for use in engineering or industrial environments.
(ii) Research Group: A second aim is to initiate, maintain and further develop a research group within a department to further and/or widen the research base. Aspects of this process include the formation of international research collaborations, appropriations of research grants, the employment of PhD's and postdoctoral researchers.

Impact

The potential impact of this current and proposed research is twofold: firstly, individual research contributions to areas within the field of computational mathematics and secondly, a new research direction to unify modelling approaches of complicated physical systems as a whole rather than splicing together ad hoc methods.