Optimised Mathematical Models for Multi-Physical Systems

Background

Environmental concerns have made it clear that there is a need for more efficient combustion engines whose combustion efficiency, and consequent reduction in greenhouse gas emissions, is greatly improved through the use of fuel sprays; recently, designed microstructures, in the form of nano-tailored surfaces have been shown to allow the possibility of the design of self-cleaning surfaces; in agriculture, 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. All of these cases involving energy/environmental engineering, nano-engineering and agriculture/biosciences represent engineering problems that are vital for the continued overall health and advancement of our technological civilisation. Fundamentally, they are all representations of phenomena which involve many different interacting physical forces acting on the interfaces where fluid-fluid and fluid-solid or elastic materials meet combining both small and large scales within one complex interacting multi-physics, multi-phase and multi-scale (MPPS) system.

To date, the interaction of multi-scale physical forces within MPPS systems is not well understood. The numerical solution of a well designed mathematical model of such problems can provide valuable insight into these interactions including better physical understanding and an ability to model systems where experiments may be too difficult or expensive to perform. One-field (OF) models allow access to a unified mathematical modelling approach of MPPS systems which is able to deal with discontinuities in material properties across interfaces and the action of interfacial/multi-scale forces such as surface tension or elasticity.

Models of physical systems, usually defined as a set of conservation laws, are sometimes solved computationally using a hybrid Eulerian-Lagrangian (HEL) numerical method. Whereas Eulerian grid based methods best capture diffusive forces such as viscosity, Lagrangian particle methods are ideal for the solution of advection equations. On the other hand, HEL methods effectively separate the system into two components, one treated in an Eulerian manner and the other in a Lagrangian way. This takes advantage of both approaches within a single method avoiding the pitfalls encountered in purely Eulerian or Lagrangian methods. The Particle-in-Cell (PIC) [1] and Marker-Particle (MP) [2] method are examples of hybrid EL methods and have been used successfully in the past to solve complex multi-phase flow problems such as droplet break-up and impact [3, 4].

Aims & Objectives

Research into the solution of multi-phase problems using HEL methods has shown that they may be the best possible way to solve such MPPS problems [5]. It is one of the aims of the proposed research to investigate this claim. Currently, the various approaches to the solution of these complex but vital multi-physics problems remain somewhat *ad hoc* since they fail to answer two fundamental questions:

- What is the best way to represent multi-scale physical forces within one-field models and avoid the development of spurious numerical artefacts, e.g. parasitic currents [5]?
- How can the Eulerian and Lagrangian components be connected without sacrificing physical principles and still maintain numerical accuracy and consistency?

It is the main aim of the proposed research to answer these two questions by reworking them as a set of three main objectives:

1. To investigate how multi-scale forces are best implemented within a one-field HEL model of a MPPS system
2. To construct one-field HEL models of MPPS systems in order to track model accuracy, convergence and stability within and between the two components
3. To construct optimal one-field HEL models of MPPS systems taking into account model accuracy, convergence, stability, efficiency and fidelity without sacrificing physical principles and mathematical consistency

My experience with HEL [2] methods and a background in analytical solution techniques [6] places me in an ideal position to resolve these issues.

Research Methodology

In order to fulfil these three objectives three different types of one-field HEL (OF-HEL) models will be considered:
Simplified - these models are simplified systems which maintain the two-component Eulerian-Lagrangian separation of a MPPS system with a minimum number of system variables e.g. the scalar advection equation
Existing - these models represent known OF-HEL models such as PIC and MP methods
Generalised - these models are generalised models representing any kind of known MPPS system

Objective 1: multi-scale forces are often upscaled where a heterogeneous medium is homogenised by imposing an effective higher scale variable which varies continuously instead of discontinuously. However, a loss of information introduced by coarsening and the small scale distribution of system variables leads to inaccuracy in large scale behaviour [7]. One advantage of OF-HEL models is that they can incorporate the effects of the unresolvable scales within the resolvable scale through the sub-grid resolution available in the Lagrangian particle component bypassing previous studies [7, 8]. This question will be investigated by analysing how well small scale behaviour is captured within the large scale by considering

- The distribution of Lagrangian particles within the Eulerian component and allocation of small scale system variables in the Lagrangian component
- The interaction of small scale system variables within the Lagrangian component and the satisfaction of conservation properties at the fine and coarse scales

This work will be assessed through comparison with known analytical results and forms the basis for the work in objectives 2 and 3.

Objective 2: the multi-scale OF-HEL models developed in objective 1 will be analysed for error transport, stability and convergence between and within the Eulerian and Lagrangian components. This analysis will be carried out using a functional analytical approach as well as numerical simulations. Typically, this involves the study of questions involving certain parameters including:

- The number of Lagrangian markers/particles used and the construction of weight/shape functions
- Which system variables should be assigned within the Eulerian or Lagrangian component
- The way boundary conditions are satisfied within both components, e.g. for mesh-free methods see [9]

This objective will develop a series of theorems describing the error growth and will form an analysis of current HEL methods. This will lay the basis for the development of optimised methods to be carried out in objective 3.

Objective 3: This objective aims to consider the models studied in objective 1 & 2 and obtain an optimised model with regard to a particular parameter, consider for example the following questions:

- What is the optimal distribution and density of Lagrangian particles within an Eulerian grid so that second order accuracy is ensured on the grid?
- What is the optimal choice of shape function which satisfies physical principles but still ensures higher order accuracy?
- What is the best way to satisfy boundary conditions within both components and maintain mathematical consistency?

These problems will be solved as constrained optimisation problems where a cost functional is assigned subject to a given constraint [10], e.g. the minimum number of Lagrangian particles subject to the constraint of second order grid accuracy.

Outcomes: The final outcome is expected to be a set of optimised one-field HEL models of typical MPPS systems which will be capable of application within commercial codes.

Timeline

My experience in HEL methods such as MP methods provides the basis for a starting point of the proposed research. This makes the construction of the Eulerian-Lagrangian models and their component variables relatively straightforward. This leads directly into objective 1 the completion of which is expected to take 6 months of the first year of the fellowship. Once the HEL models have been properly defined they are amenable to error analysis which is the basis of objective 2 which is expected to take the remainder of the first year of the fellowship. The last objective will be the most intensive and is assigned the second year of the fellowship.

References

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