Chapter 4

Summary and Conclusions

In this thesis a numerical method has been presented for simulating fluid flow under micro-gravity conditions and for the simulation of coupled solid-liquid dynamics. The numerical model has been implemented in a computer program called ComFlo with which all the simulations in this thesis have been performed.

Computational Grid

In chapter 2 a numerical method for discretising the Navier-Stokes equations on a three-dimensional, Cartesian grid was introduced. On a Cartesian grid it is relatively easy (compared to an unstructured grid) to advect a free surface. Further, grid generation becomes a trivial task compared to the generation of a body-fitted grid, which can be extremely time consuming.

For incorporating complex geometries the cut-cell technique was used, meaning that the boundary of the solid body cuts the Cartesian grid, hereby creating small, irregular grid cells. The representation of a complex geometry on a Cartesian grid was accomplished by introducing apertures, which indicate that part of a cell and its cell faces may be closed for flow. Simulation of wall-adhesion flow in a circular cylinder showed that use of the cut-cell technique is crucial for simulating fluid flow in complex geometries. Indeed, the same simulation in a staircase approximation of the circular cylinder gave deviant and incorrect results.

Discretisation Method

The finite-volume method was used for the discretisation of the Navier-Stokes equations. Thus, a weak formulation of the governing equations was the starting point for the numerical method. In the discrete approximations of the divergence and gradient operators apertures were included to account for complex geometries. The discretisation was done such that the discrete operators for convection and diffusion have the same symmetry properties as their continuous counterparts, *i.e.* the discrete operator for convection is a skew-symmetric matrix and the discrete operator for diffusion is a symmetric, negative-definite matrix. Further, the discrete gradient operator is equal to minus the transpose of the discrete divergence operator. From these symmetry properties it follows that, in the absence of external forces, the kinetic energy of the flow can not grow, making the numerical method extremely robust.

The discrete Navier-Stokes equations seem quite complex because of the inclusion of apertures and the incorporation of stretched grids. However, when applied to a staircase-shaped geometry on a uniform grid, the spatial discretisation reduces to a familiar, second-order finite-difference discretisation.

Despite the presence of small cells, no severe limitations on the time step were encountered. In fact, it can be proven that the discretisation of the convective terms that was exploited in this thesis leads to a time-step restriction that is based on the mesh size of the Cartesian grid; small cells do not make this restriction more stringent. Diffusive terms do strengthen the time-step restriction. However, by using a lower limit for the size of control volumes for discretising diffusion, this limitation is kept within bounds. Effectively, this precaution shifts the solid boundary over a small distance (smaller than the size of a computational cell) before applying the no-slip boundary condition.

Free-Surface Advection

Another focal point of chapter 2 is the numerical method for simulating interface flow. Two methods for interface advection were studied, namely the method of Hirt and Nichols and of Youngs. In the method of Hirt and Nichols the interface is reconstructed piecewise constant (thus, aligned with the Cartesian directions). The reconstructed interface is advected using limiters to prevent large undershoots and overshoots in the VOF function and to prevent unwanted steepening or smearing of the interface. In the method of Youngs a piecewise-linear reconstruction of the interface is computed. Based on the reconstructed interface, fluxes are computed which are transported unchanged from a donor cell to an acceptor cell. It was shown that both advection methods have severe problems with mass conservation. Moreover, the method of Hirt and Nichols creates a lot of flotsam and jetsam. The problems encountered in both advection methods can be solved by introducing a local height function near the free surface. In every surface cell, locally a height function is defined in a 3×3 (two dimensions) or $3 \times 3 \times 3$ (three dimensions) block of grid cells. The fluxes that have been computed at cell faces are not directly transported from a donor cell to an acceptor cell, but instead the value of the local height function is updated. This method for advecting the free surface conserves mass rigorously and creates far less flotsam and jetsam.

In fluid-flow problems with a prescribed velocity field, the use of a local height function improves the method of Hirt and Nichols a lot, while Youngs' method is less beneficiary. In these problems Youngs' method (with or without a height function) performs superior. However, in simulations where the velocity field is solved from the Navier-Stokes equations, Youngs' method (with or without a height function) gives worse results than the method of Hirt and Nichols combined with a local height function. This is due to the linear reconstruction of the interface. For this, the normal of the interface is predicted using the VOF field around the cell under consideration. Since the velocity field is computed up to a user-defined accuracy, small errors occur in the distribution of the VOF field, for which the computation of the normal, and thus the entire advection algorithm, is very sensitive. Typically, Youngs' method loses symmetry quickly in symmetrical flow problems. The method of Hirt and Nichols is not sensitive to small variations in the VOF field since the interface is reconstructed piecewise constant. Therefore, the method of Hirt and Nichols combined with a local height function is preferred in this thesis.

Micro-Gravity

In this thesis, capillary forces, such as surface tension and wall adhesion, could not be neglected since a numerical model was needed for the simulation of liquid dynamics in space. Therefore, the boundary conditions at the free surface required much attention. Especially, a correct implementation of the boundary conditions for the pressure and the contact angle is crucial for obtaining accurate results. Indeed, in the various wall-adhesion simulations described in this thesis, the contact angle and surface tension drive the flow and determine the steady-state solution. The pressure at the free surface depends on its curvature, which is computed using the local height function that was introduced earlier for advecting the free surface. By means of grid refinement and comparing results from simulations (with various contact angles) to theory, the numerical method has been validated. In two dimensions, both in simple and complex geometries, the results agree closely. The three-dimensional simulation of wall adhesion in a sphere showed that the free surface is not perfectly axisymmetric. However, the steady-state solution is adequately predicted considering the fact that all the information in these simulations comes from the contact line, which is a one-dimensional subset of the flow domain.

Coupled Dynamics

The model that has been developed in chapter 2 was extended in chapter 3 by coupling the liquid dynamics with the dynamics of the solid body in which the liquid is contained. This required a model for the solid-body dynamics in which terms appear representing the force that the sloshing liquid induces on the solid body. Further, the model for the liquid dynamics was extended with a virtual body force accounting for the solid-body motion.

The governing equations for the solid-body dynamics are naturally written with respect to an inertial reference frame. Hence, also the force due to the sloshing liquid is written with respect to this reference frame. However, discretisation of these equations results in a numerical method that is unstable if the liquid mass becomes too large with respect to the mass of the solid body. This is demonstrated in a simulation of the free fall of a liquid-filled container. This stability problem was solved by writing the sloshing force as a sum of two contributions. The first contribution is the force resulting from linear and angular accelerations of the fluid, due to motion of the solid body. The second contribution is the force due to accelerations of the fluid with respect to the moving reference frame. The former contribution is then treated simultaneously with the motion of the solid body. Discretisation of this alternative mathematical model for the solid-body dynamics results in a numerical model that is stable for arbitrary liquid/solid mass ratios. This unconditional stability was exemplified with a mass-spring model and demonstrated with simulations where the liquid/solid mass ratio ranged from 0.1 to 100.

Flat Spin

An important example of coupled solid-liquid dynamics is the flat-spin motion of a (partially) liquid-filled spacecraft. In this case the coupled system is initially rotating around its axis with minimum moment of inertia. From physics it is known that a free-flying body can rotate uniformly around one of the three principal moment-of-inertia axes only;

rotation around the axis with intermediate moment of inertia is unstable, while rotation around the other two axes is stable. Thus, the initial condition (rotation around the axis with minimum moment of inertia) can be a steady state. However, if damping in the coupled system occurs (*e.g.* due to the viscous liquid), kinetic energy is lost. Hence, in this case, rotation around the axis with maximum moment of inertia (corresponding to a state of minimum kinetic energy) is the steady state in which the coupled system settles itself. A flat-spin motion of a three-dimensional, rectangular container partially filled with liquid has been simulated. This simulation showed that the numerical method can predict a flat spin correctly. A quantitative comparison of a flat spin was made by simulating the Wet Satellite Model (WSM) experiment, which was performed in space in 1992. In fact, ComFlo is the first computational fluid dynamics method that performed a simulation of the WSM experiment. Although the geometry of the WSM (a thin annulus) is not very suitable for a numerical method based on Cartesian grids, results of the simulation agree adequately with the experiment.

Epilogue

From the results of the various simulations that have been discussed in this thesis (and from the many more simulations that have been performed in developing the numerical method, but are not reported here), it can be concluded that the present method is capable of simulating liquid dynamics under micro-gravity conditions and can predict the coupled dynamics of liquid-filled spacecraft. The method is very robust and applicable for simulation of terrestrial fluid-flow problems as well. However, for further (physical) understanding of liquid behaviour in space — especially with respect to contact-line dynamics — and validation of numerical methods, experiments remain extremely valuable. Hence, the forthcoming launch of the experiment satellite SloshSat FLEVO will hopefully be a success and help in the further development of micro-gravity computational fluid dynamics.