

# **A new unstructured algorithm based on the Volume of Fluid method for tracking material interfaces in a finite-volume framework**

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## **ABSTRACT**

*In recent years significant effort has been put in developing various numerical techniques for the study of flows that involve convoluted material interfaces. One of the most successful techniques has been the Volume of Fluid (VOF) method, developed in the late seventies-early eighties at Los Alamos [1]. The VOF method uses an Eulerian approach and relies on the calculation of a scalar parameter, representing the fractional volume of fluid in a numerical cell, in order to track interface distortions. This scheme's popularity is based on its ease of implementation, its accuracy and its computational efficiency. A number of techniques based on VOF have been developed over the past twenty years for a number of applications, as diverse as tracking water droplets caught in an air stream and polymer mould filling, see e.g. [2]). Unfortunately, all these techniques have been developed for structured meshes and follow the finite-differences discretisation of the*

*original scheme. Recently, attempts have been made to construct VOF schemes in FE frameworks. However, these employ secondary structured grids for the solution of the scalar advection equation for the tracking of the material interface [3].*

*In the present paper the construction of an unstructured VOF scheme and its implementation in a 3-D finite volume framework is discussed. The capabilities of the scheme to maintain sharp material interfaces and minimise numerical diffusion and subsequent loss of momentum are then demonstrated through a series of numerical tests and simulations.*

**KEY WORDS:** VOF, Volume of Fluid, Interface Tracking, Sharp Interfaces, and PHYSICA

#### **INTRODUCTION**

The accurate prediction of air-liquid interfaces is a key component in the numerical modelling of a number of processes. For example

- (1) Casting [4], the process involves free surface flows as the mould fills and is coupled with a number of other processes (Convection, Heat Transfer and Solidification) and
- (2) Hopper filling/emptying [5], the process involves the charging and discharging of hoppers containing granular material and is coupled with a number of other processes (Segregation, Degradation, and Caking).

The need for unstructured meshes is necessary in order to simulate problems that involve convoluted interfaces in geometries where their complexity is an integral part of the simulated problem. This is especially true in the vicinity of flow boundaries, to accurately represent the problem's geometrical features and associated physical interactions of the boundaries to the flow. The emptying / filling of hoppers with particulate materials and liquid metal casting simulations may be offered as examples of such cases, where interface phenomena in the vicinity of complex geometrical boundaries determine the further evolution of the flow.

#### **MODELLING FRAMEWORK**

The full set of flow equations were solved using PHYSICA, a finite-volume code developed at the University of Greenwich [6]. The PHYSICA toolkit is a three-dimensional, fully unstructured-

mesh modular suite of software for the simulation of coupled physical phenomena. Choices of differencing schemes (i.e. central differencing, upwinding, hybrid, power law, exponential) are available. Furthermore, the Rhie-Chow interpolation method [7] is employed to avoid the possibility of checkerboard velocity and pressure fields. SIMPLE-based algorithms are used for the solution of the flow equations; see e.g. [8] together with the option of a number of iterative solvers (i.e. conjugate gradients, Gauss-Seidel, Jacobi) may be invoked for the numerical solution of the discretised equations. A range of turbulence models, source-based solidification/melting algorithms and elasto-visco-plastic solid mechanics models are also an integral part of the framework. Finally, PHYSICA has been successfully applied to a number of problems involving complex interactions of physical behaviour over arbitrarily unstructured domains; see e.g. [9-10].

#### COMPUTATIONAL MODEL

The interface tracking computational model utilised for the current study is based a modified version of the commonly used Volume of Fluid tracking approach. The recently developed approach, available in PHYSICA, is termed UDA-VOF, which stands for Unstructured-Donor-Aceptor VOF algorithm. Here the UDA-VOF is different to the standard VOF technique in that the interface is reconstructed from arbitrary shaped control-volumes to determine the interface direction through calculation of the  $F$ -function fluxes across control-volume surfaces. Indeed, in the standard VOF approach, “Free-Surface” cells are only employed to re-construct the interface. This introduces a substantial level of numerical diffusion and results in smeared interfaces. In the UDA-VOF scheme, the directional gradients of the  $F$ -function are calculated by considering all elements containing liquid and “Free-Surfaces”. Information from upstream and downstream of an element is used to determine the interface orientation within all the liquid elements. This helps account for the voids present within the liquid cell. Voids are filled on a “first-come-first” basis, thus ensuring accurate pressure and velocity calculations and the loss of liquid momentum is minimised. This ensures that a sharp interface is maintained without need of artificial numerical corrections.

The governing equations for modelling the types of examples that follow are as follows:

**Volume of fluid equation:** 
$$\frac{\partial F}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial w}{\partial z} = 0$$

**Energy equation:** 
$$\rho c \frac{\partial T}{\partial t} + \rho c u \frac{\partial T}{\partial x} + \rho c v \frac{\partial T}{\partial y} + \rho c w \frac{\partial T}{\partial z} = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + S$$

**Continuity equation:** 
$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

**Navier-Stokes equation:**

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} &= -\frac{1}{\rho} \frac{\partial p}{\partial x} + g_x + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} &= -\frac{1}{\rho} \frac{\partial p}{\partial y} + g_y + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) \\ \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} &= -\frac{1}{\rho} \frac{\partial p}{\partial z} + g_z + \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) \end{aligned}$$

where  $t$  is the simulation time,  $\rho$  is the density,  $c$  is the specific heat,  $u$ ,  $v$  and  $w$  are the velocity,  $p$  is the pressure,  $g$  is the gravitational acceleration,  $k$  is the thermal conductivity,  $F$  is the volume of fluid and  $\mu$  is the dynamic viscosity.

#### NUMERICAL SIMULATIONS AND MODEL TESTING

##### EXAMPLE 1: WATER SLUMPING CASE

The water slumping case involves the simulation of a square of heavy liquid that falls under the influence of gravity, Figure 1. Experimental data have been reported; see Martin and Moyce [11], for a variety of base width to column height ratios, for rectangular and circular cross section columns. For the present study, only 2-dimensional simulations are considered, thus due to symmetry only the rectangular cross section data are compared. Figure 2 present graphs for the base width to column height ratios of 1 and 2 respectively. Normalised distance of the column along the base plane,  $z/a$ , against normalised time,  $nt(g/a)^{1/2}$ , where  $a$  is the base width of the column,  $g$  is gravity and  $n^2$  is the ratio of column height to width are plotted. The predicted results are in excellent agreement with experimental data.

##### EXAMPLE 2: HOLLOW SQUARE CASE

This case involves the simulation of a square shaped block of a dense fluid falling through a lighter fluid under the influence of gravity. The central core of the dense block contains lighter fluid. After falling a distance the square impacts on a bath of the denser material. A schematic of the case can be seen in Figure 3. The case tests the ability of the free surface algorithm to maintain the shape of the hollow cube. One of the major difficulties of this case is the handling of the

pressure gradient term across the material interfaces, both internal and external, of the square. Any inaccuracies in the calculation of the gradients would have lead to the break-up of the square before impacting the stationary liquid. The numerical results, presented in Figure 3, show that the shape of the square is maintained throughout the duration of the fall and it only distorts once it comes in contact with the still lighter fluid. The lower front of the square breaks upon impact with the lighter fluid. The reaction wave generated by the entry of the heavier fluid is also clearly visible in the later stages of the simulation.

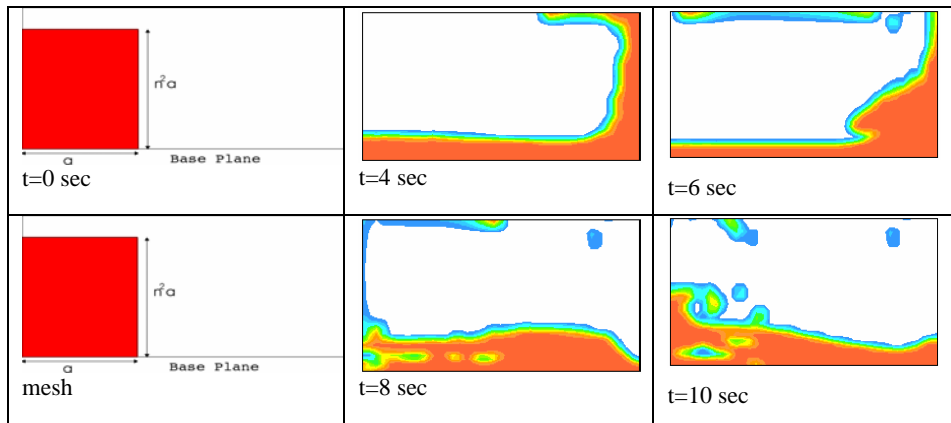


Figure 1: Initial condition, Mesh and Interface configuration for water slumping problem

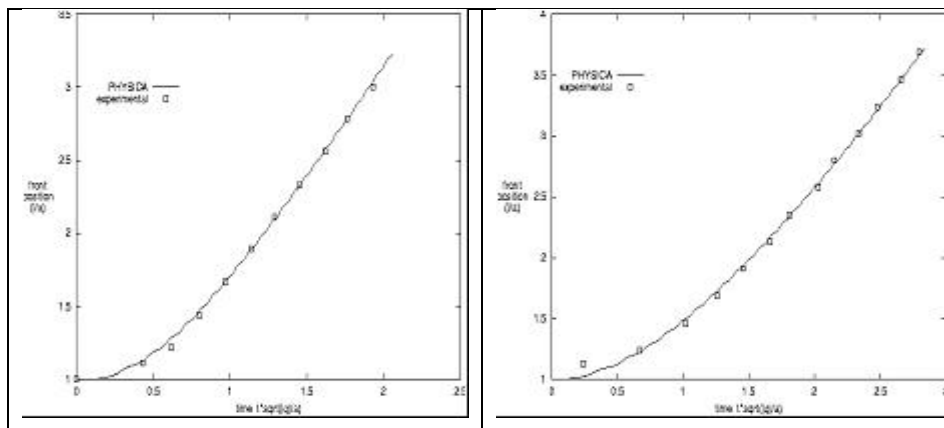


Figure 2: Comparison of the predicted vs. experimental data for (a) 1x1 and (b) 2x1 column

### EXAMPLE 3: FLOW THROUGH A PIPE

This case tests the performance of the interface-tracking algorithm for a triangular unstructured grid. Gravity-driven flow. Dimensions of pipe: 2 m by 5 m. The domain is initially filled with water, which is replaced by air as the pipe empties. The mesh is shown in Figure 4 together with the evolution of the interface at various time-steps. In spite of the unstructured mesh, the liquid interface remains well defined and the smearing is limited within one neighbouring cell. Indeed, the agreement of the results compare well with the propagation speed of velocity x timestep.

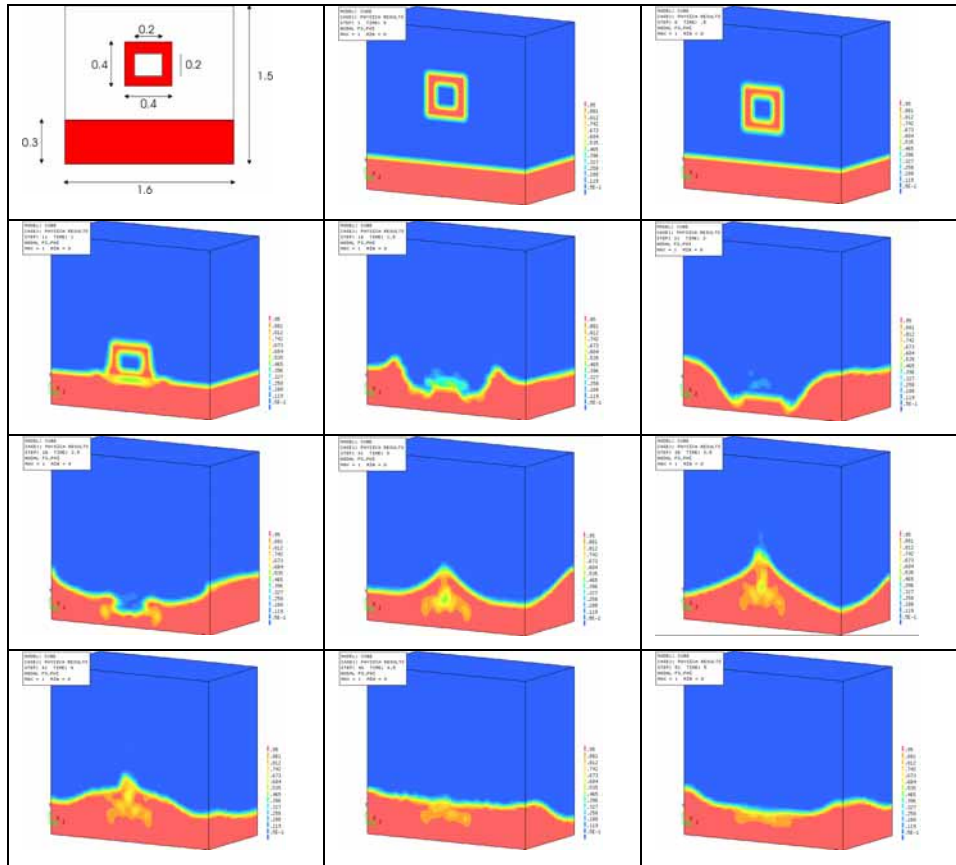


Figure 3: Initial condition, Mesh and Interface configuration for water slumping problem

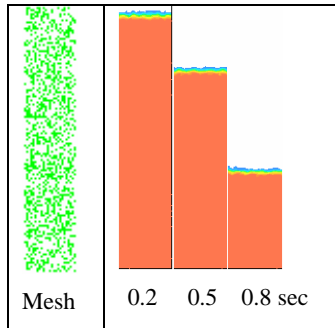


Figure 4: Mesh and Interface configuration for flow through a pipe

#### SUMMARY

The paper demonstrates the successful use of the UDA-VOF technique to predict the interface movement within air-liquid, fluid flow problems. The robustness of the approach have been assessed by the use of a number of complex unstructured meshes, all of which managed to yield acceptable results. The results presented here are a selection of those obtained. Indeed, it can be concluded that for problems that require the tracking of an interface, the new approach works well and should lend itself well to large-scale practical problems. The method managed to maintain very sharp interfaces, in unstructured meshes, without the need for artificial corrections. In most cases, the smearing was limited well within neighbouring cells. It is worth noting that even without the explicit representation of turbulence, the agreement of the water slumping case is very good.

The next phase of the on-going work to will consider the extension of the technique to three-dimensions with further validation/verification for coupled problems that include solidification.

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