The Immersed Surfaces Technology for Reliable and Fast Setup of Microfluidics Simulation Problems

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ABSTRACT

In many microfluidic applications, the complexity of the system is such that it requires tremendous efforts to setup the CFD problem, ranging from dimensioning of the computational domain, to grid setup. In setting up a grid, the user must complain to various constraints: adequate near-wall resolution, reduce the aspect ratio and the rate of grid stretching, and control of cell skewness (in the framework of BFC structured grids). These issues can cause a large amount of numerical diffusion errors, which in turn requires reducing convection scheme accuracy to 1st-order to avoid divergence of the solution. We present here a new technique based on immersed surfaces that alleviates most of the evoked problems with traditional grid generation, permitting reliable and fast setup of microfluidics problems.

Keywords: Microfluidics, CFD, IST, BMR, Interfacial flow

1 INTRODUCTION

As bio-chips may comprise various components (multi channels and components, complex configurations), we have developed a new fully automatized version for microfluidics applications in bio-devices, using the IST (Immersed surfaces Technique) technique to map complex components/geometries into a simple rectangular Cartesian grid. In such a way, the drawbacks of traditional girding are alleviated: aspect ratio, cell stretching and skewness.

IST forces the grid to remain Cartesian and equidistant in all directions, thus high-order schemes (we use up to 3rd order for flux convection and 3rd order WENO schemes for free surface flows) can maintain their high degree of accuracy. Further, to better resolve boundary-layer regions, near wall flow areas are treated by another new feature, namely the BMR (Block-based Mesh Refinement), in which sub-scale refined blocks are placed around each structure or obstructions. The connectivity between blocks can be achieved in parallel (using MPI) up to 8-to-1 cell mapping. The combination IST/BMR can save up to 70% grid cells in 3D. In this paper we report examples of microfluidics bio-devices treated with this approach, without dealing in detail with the flow results. The flow physics simulated by the code TransAT of similar problems is detailed in our companion paper (this volume [1]).

2 INTERFACE TRACKING FOR MICROFLUIDCS FLOW PROBLEMS

Interfacial flows refer to multi-phase flow problems that involve two or more immiscible fluids separated by sharp interfaces which evolve in time. Typically, when the fluid on one side of the interface is a gas that exerts shear (tangential) stress upon the interface, the latter is referred to as a free surface. Interface tracking methods (ITM) are schemes capable to locate the interface, not by following the interface in a Lagrangian sense (e.g., by following marker points on the interface), but by capturing the interface by keeping track, in an Eulerian sense (the grid is fixed), of the evolution of an appropriate field such as a level-set function or a volume-fraction field. Examples and classifications are provided in [2]. Application of ITM's to microfluidics flows requires further attention to the way surface forces are handled.

2.1 TransAT© Microfluidics Flow solver

The Microfluidics code TransAT© [3] of ASCOMP is a multi-physics, finite-volume code based on solving multi-fluid Navier-Stokes equations on structured multi-block meshes. MPI parallel based algorithm is used in connection with multi-blocking. Grid arrangement is collocated and can thus handle more easily curvilinear skewed grids. The solver is pressure based, corrected using the Karki-Patankar technique for weak compressible flows. The Navier-Stokes and level set equations are solved using the 3rd order Runge-Kutta explicit scheme for time integration. The convective fluxes are discretized with TVD-bounded high-order schemes [4]. The diffusive fluxes are differenced using a 2ndorder central scheme.

Multiphase flows are tackled using Level Sets and VOF for both laminar and turbulent flows. The solver incorporates phase-change capabilities, surface tension and triple-line dynamics models, Marangoni effects, and a micro-film sub-grid scale model for lubrication. 3D flows are treated using the IST to map the components into a simple rectangular Cartesian grid. BMR helps refine grids around the flow areas of interest, up to 1-to-8 level connection between the blocks, as explained below. Details of the modeling of interfacial flows can be found in [1].

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2.2 Predictive Performance of ITM's

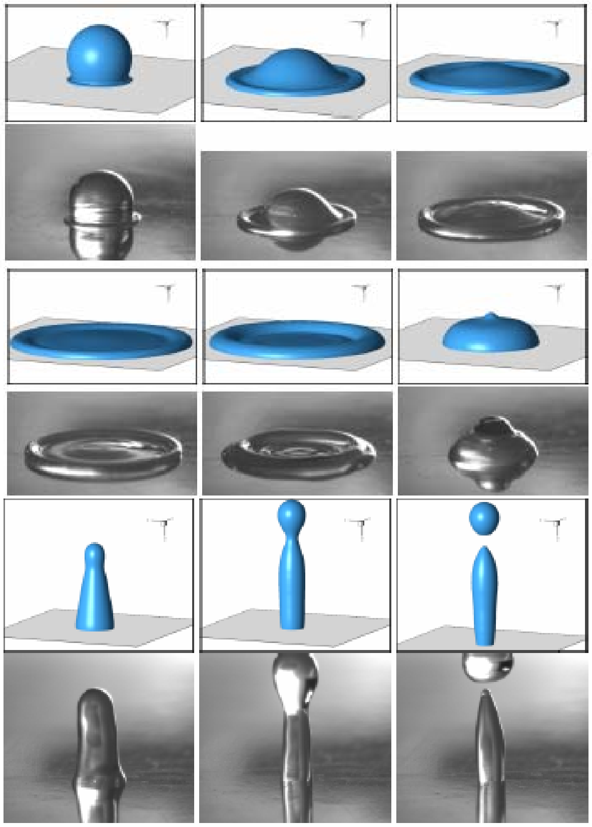

Figure 1: Partial bouncing of microdroplets on a dry surface obtained for CA = 100, We= 52 and Re = 3245 [5]. CFD results (surface level sets in blue) vs. experiments (grey).

Figure 1 above illustrates the predictive performance of the ITM's methods (Level Sets [6]) implemented in TransAT for treating contact-angle driven flows. The bouncing or splashing of liquid droplets on dry surfaces is mainly dependent on the contact angle (CA), Weber and Reynolds number (We and Re), and surface roughness (in this example the surface is smooth). The comparison between the data and TransAT simulations is perfect, including for 3D splashing and bouncing; see detailed comparison in [5].

3 IMMERSED SURFACES TECHNIQUES WITH BLOCK MESH REFINEMENT

The Immersed Surfaces Technology (IST) has been developed at ASCOMP GmbH, although other similar approaches have appeared in parallel. The underpinning idea is inspired from ITM's for two-phase flows (VOF and Level Sets), where free surfaces are described by a convection equation advecting the phase color function.

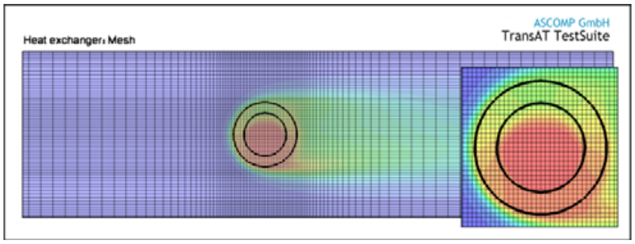

Figure 2: Representation of the tube, $\phi_s = 0$, within IST.

In the IST solid surfaces are described as the second 'phase', with its own thermo-mechanical properties. This new technique differs substantially from the Immersed Boundaries methods [7], in that the jump condition at the solid surface is implicitly accounted for, not via direct momentum forcing on the Eulerian grids. It has the major advantage to solve conjugate heat transfer problems, in that conduction inside the body is directly linked to external fluid convection.

The air-coolant flow past a circular tube half-filled with hot liquid shown in Figure 2 is an illustrative example. The solid is first immersed into a Cartesian mesh. The solid is defined by its external boundaries using the solid level set function, ϕ_s. Like in fluid-fluid flows, ϕ_s function is defined as a distance to the surface; is zero at the surface, negative in the fluid and positive in the solid. The treatment of viscous wall shear is handled as in all CFD codes; wall cells are identified as those in which $0 < \phi_s < 1$. The figure shows the grid and the heat transfer resulting from the coupled convection-conduction; the coolant air from the left removes heat from the tube walls, first convected within the liquid in the tube, then conducted through the tube walls.

4 MICROFLUIDCS GRID SETUP TESTS

4.1 Fluid Handling in a Micro-reactor

Micro-reactor chips consist of an array of on-chip fluid handling modules, and are used as "liquid circuit boards" that can be configured for a variety of biochemical and cell-based assays including: drug formulation, on-chip chemical synthesis and screening, reagent mixing, etc.

The test case presented below is an idealized set-up (Fig. 3), consisting of two inflow sections from which a liquid train (e.g. reagent) is injected, which later on breaks up into micro-droplets. These should coalesce in the center and exit from below. Such systems may enable rapid screening of a wide range of cells and molecules under a variety of assay conditions in a very cost effective way, compared for example to manual manipulation using for instance robotic microliter plate systems. Fast response of CFD here can be invaluable for large data-basis treatment.

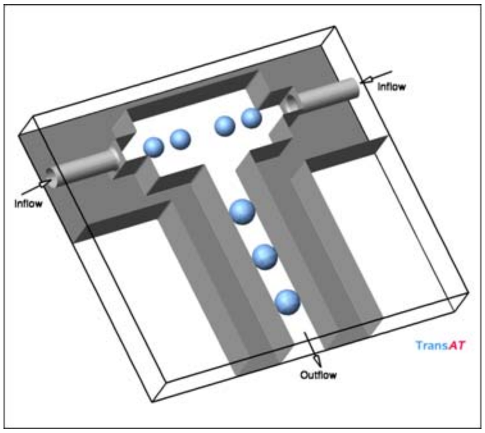

Figure 3: An idealized configuration of a micro-reactor.

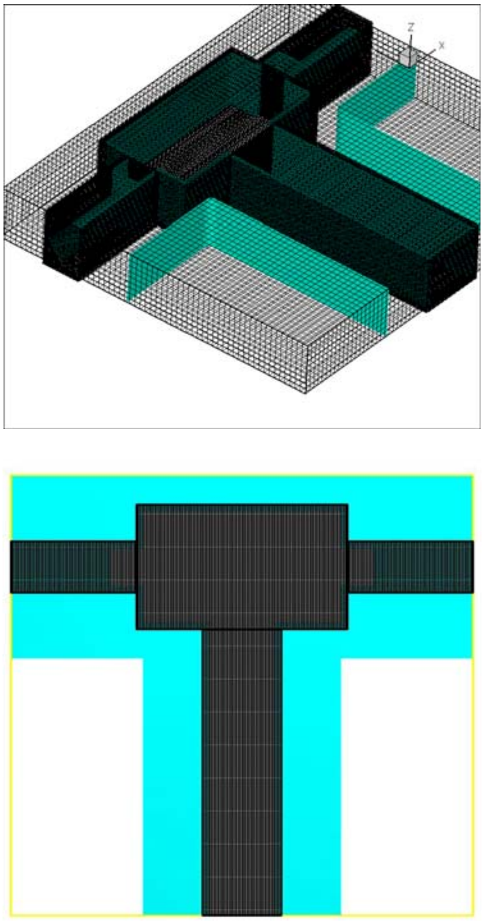

Figure 4: Step 1, cover the domain with a 1st grid. Step 2: create refined blocks then remove the coarse grid.

We start by importing the CAD file representing the systems from a library. The file is then loaded and will be automatically entirely covered by a 3D Cartesian mesh (Fig. 4). The microfluidics code TransAT recognizes all solid surfaces as the zero level of the solid level set function, as well as the number of blocks contained in the CAD file. A coarse grid covers first the entire domain (Fig. 4), and then refined blocks are added automatically in the tubes and channels. Finally the coarse grid is removed.

4.2 Cardiovascular Gas Bubbles in Arterial Y-Junction Bifurcation

Cardiovascular gas bubbles in arteriole bifurcations (Fig. 5) have been experimentally addressed to understand the dynamics of their lodging mechanism [8]. The research is motivated by novel gas embolotherapy techniques for the potential treatment of cancer by tumor infarction; the findings may be useful in developing strategies for microbubble delivery in gas embolotherapy. A prototype has been set as a challenging example for the IST/BMR technique of TransAT. The physics of the flow itself is very complicated, requiring in particular the inclusion of sub-grid ultra thin film in the model (built within the ITM strategy) to avoid numerical breaking of the film as it approaches bifurcation corner. The model developed for the purpose is explained in the companion paper, together with selected results.

The same procedure alluded to previously is repeated here to mesh the Y-junction bifurcation shown in Fig. 5 below. The case represents the situation where a liquid slug may either travels within one branch of the junction, or breaks at the junction corner. Again we start by importing the CAD file of the systems from a library (Fig. 6). The file is then loaded and will be automatically entirely covered by a 3D Cartesian mesh (Fig. 7a). The microfluidics code TransAT recognizes all solid surfaces as the zero level of the solid level set function, as well as the number of blocks contained in the CAD file. BMR refined blocks are then automatically generated around the three branches. Finally the coarse grid can be removed (Fig. 7b). The entire procedure lasts less than 30 minutes; the fluid dynamics simulation time depends on the available computing power.

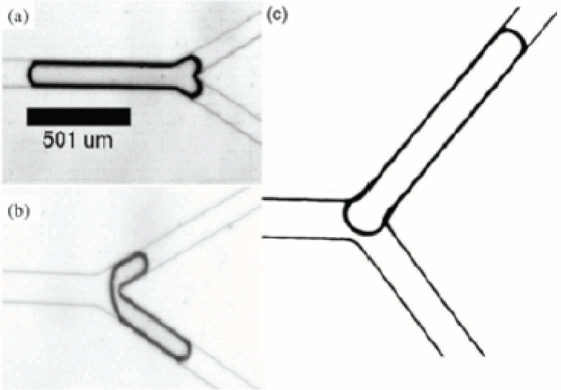

Figure 5: (a) Lodging state, (b) Lodging state, (c) Bubble lodged in one of the branches [8].

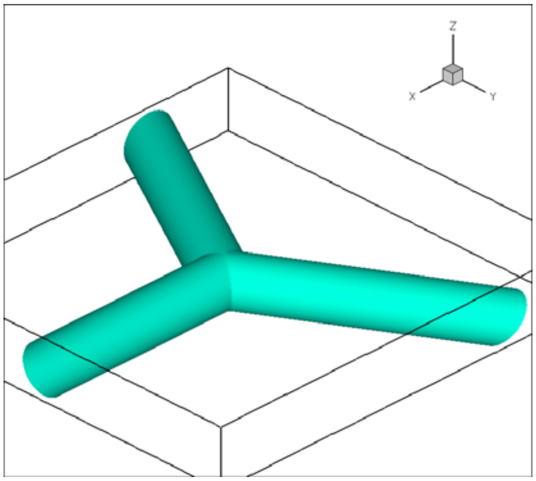

Figure 6:An idealized configuration of Fig. 5.

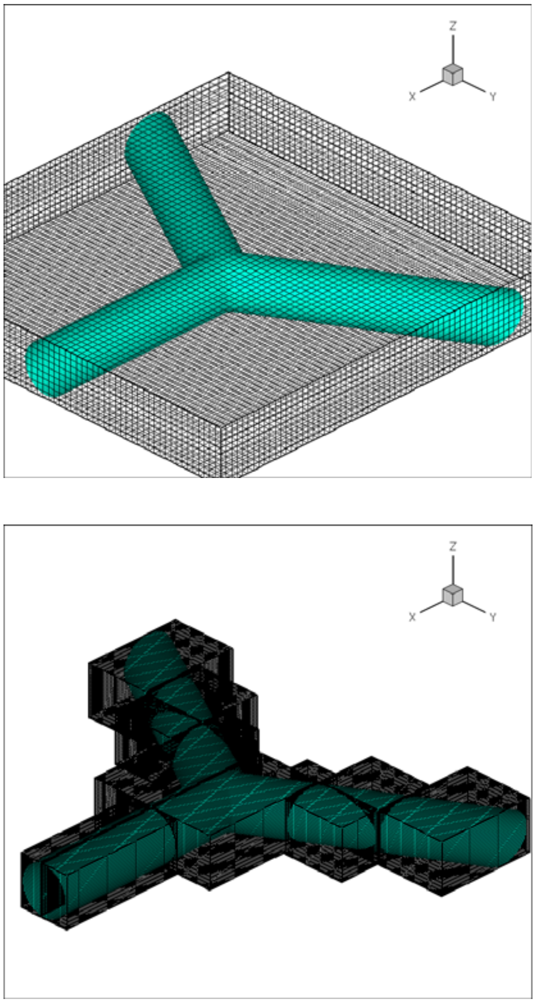

Figure 7: Step 1, cover the domain with a coarse grid. Step 2: Create refined BMR blocks around the braches and remove the coarse grid.

4.3 Liquid Filling of a Lab-on-Chip

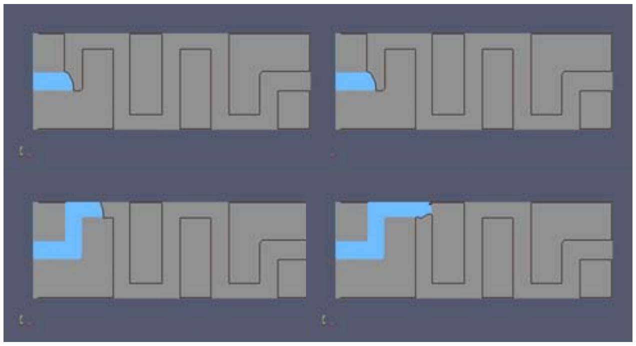

Figure 8: 2D filling of a lab-on-chip by a liquid (CA=90)

The example shown in Fig. 8 above corresponds to the microfluidic filling in lab-on-chip channels (in 2D). The setup of the grid is as explained in the two previous examples; here we present snapshots of the simulated flow (using the Level Set approach). The objective here is to analyse the possibility of small air bubbles entrapment in the cavities, depending on the surface wettability (contact angle). This phenomenon can only be simulated with appropriate wetting modelling of the triple line dynamics, as explained previously; here the contact angle is set statistically to 90 deg.

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