Computational Modeling of Fluidic Micro-Handling Processes

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ABSTRACT

This paper describes the application of a new and unconventional numerical method for computational modeling of fluidic micro-handling processes. The key requirement for modeling such processes is the ability to simulate flows with large number of complex shaped moving objects. Conventional body-conformal computational fluid dynamic (CFD) methods are not well suited for simulating such flows and here we have employed a new Cartesian Grid Method (CGM) which has the unique ability of simulating these complex flow on stationary Cartesian grids. The method has been used to simulate a generic fluidic assembly process and is shown to predict some interesting features of this process.

Keywords: microflows, computational fluid dynamics fluidic micro-handling, Cartesian grid methods, microassembly.

1 INTRODUCTION

One key feature that characterizes the assembly of microsystems is the need to "handle" a large number of microcomponents. Handling may for instance include transport of a microcomponent from one location to another, orientation control and sorting. Furthermore, the process employed in the assembly should be highly scalable in order to be able to mass produce the microsystem in a cost-effective manner. Conventional 'pick-and-place' technologies are unsuitable for many microsystems due the difficulty in handling small size components and in scaling up these techniques for mass production. Unlike top-down approaches to conventional manufacturing that are amenable to pick-and-place techniques, the bottoms-up approach needed in the assembly of microsystems requires a fundamentally different point-of-view

Fluidic transport provides a powerful means for handling of component in many microsystems and is increasingly being employed in a number of such applications. One of the first commercialization of such a process is the so called Fluidic Self-Assembly (FSA™ Alien Technology Corp.) process which is being employed for the assembly of flat panel displays. In this process, specifically shaped semiconductor devices (see fig. 1) ranging in size from 10 microns to several hundred microns are suspended in liquid and flowed over a surface which has correspondingly shaped receptor sites on it into which the devices settle. The shapes of the devices and the receptor sites are designed so that the devices fall easily into place and are self-aligning. One key feature here is that the components that are transported are of a variety of shapes and the shape of these components strongly affects how they are transported in a fluid. Thus factors such as speed of transport and orientation of the transported components which are all important in this process, are highly dependent on the shape of the components. Thus techniques employed in computational modeling of conventional particulate flows where particles are almost always modeled to be spherical in shape, would be of limited use for a process such as FSA™. Other examples of the use of fluid transport in micro-handling include air based micro-conveyance systems [1] and fluidic assembly of cells in biomedical applications.

(a) **(b)**

Figure 1. (a) Geometry and typical size of NanoBlocks™ (b) Schematic showing NanoBlocks™ on substrate. Figures provided courtesy of Alien Technology Corporation.

In addition to this, there are other applications where fluid transport is not the primary handling agent but the transport is nevertheless affected by fluid flow. An example of this is the assembly process of RF-ID tags being developed at the Auto-ID Center at MIT (http://www.autoidcenter.org/main.asp). In this vibratory based transport system, the last phase involves the microcomponent falling through air onto a receptor site on a moving conveyor belt. The motion of the conveyor belt induces a flow which in turn can affect the motion of the microcomponent as it falls through the air. Thus precise placement of the component into the receptor site would be significantly assisted if the fluid flow effects on the component can be understood. Finally, in the future we can envision other systems based upon powered fluidic devices such as synthetic jets for more precise handling of micro-components which would require detailed understanding of the fluid flow aspects.

Thus computational modeling of fluidic micro-handling processes requires numerical techniques that have the ability to simulate the transport of a large number of distinct bodies where the shape and orientation of the each body is reasonably well represented. Conventional body-conformal structured or unstructured grid methods would require enormous resources and would also entail significant complexity due to the need to fit a new grid around hundreds of complex moving shaped bodies at each time step of the simulation. For such simulations, methods that simulate the flow on simple, fixed Cartesian meshes [2] offer a much more viable alternative. The advantage of these methods is that the complexity and cost of generating a body-conformal mesh at each time-step is eliminated, thereby easing the resources required to perform such simulations. These methods are not well suited for high Reynolds number flows due to their inability to provide resolution in localized regions such as boundary layers. However, in fluidic micro-handling processes, the Reynolds numbers based on the component sizes are quite small and thus the Cartesian grid methods are not at any disadvantage in such applications.

In the current paper, we present the applications of a Cartesian grid method to a modeled problem associated with the FSA™ process. The results are intended to display the potential of this method for such applications.

2 NUMERICAL METHOD

The framework of the method developed in these papers is Eulerian-Lagrangian, i.e. the immersed boundaries are explicitly tracked as curves in Lagrangian fashion, while the flow computations are performed on a fixed Eulerian mesh. This affords the advantage of pure Lagrangian methods such as explicit interface information without ambiguities associated with *a-posteriori* reconstruction of the interface from an advected scalar (such as Volume-of-Fluid, Level Set or phase field). However, we dispense with mesh movement and thereby circumvent some of the problems associated with mesh management. In contrast with purely Eulerian interface capturing approaches (diffuse interface methods) the current method treats the immersed boundaries as sharp interfaces. The distinguishing feature of the present method is that the governing equations are discretized on a Cartesian grid which does not conform to the immersed boundaries. This greatly simplifies grid generation and also retains the relative simplicity of the governing equations in Cartesian coordinates. Therefore, this method has distinct advantages over the conventional body-fitted approach in simulating flows with moving boundaries, complicated shapes or topological changes.

2.1 Interface Tracking

The interface is tracked using markers connected by piecewise quadratic curves parametrized with respect to the arclength. Details regarding interface representation, evaluation of derivatives along the interface to obtain normals, curvatures etc. have been presented in previous papers [2,3] and are not repeated here. Also described in earlier papers are details regarding the interaction of the interfaces with the underlying fixed Cartesian mesh. These include obtaining locations where the interface cuts the mesh, identifying phases in which the cell centers lie, and procedures for obtaining a consistent mosaic of control volumes in the cells. This results in the formation of control-volumes which are trapezoidal in shape as described in [3].

2.2 Flow Solver

The fractional step scheme[3] is used for advancing the solution in time. The Navier-Stokes equations are discretized on a Cartesian mesh using a cell-centered colocated (non-staggered) arrangement of the primitive variables (***u***,*p*). The integral form of the non-dimensionalized governing equations are used as the starting point:

$$\oint \vec{u} \cdot \vec{n} dS = 0 \tag{1}$$

$$St \frac{\partial}{\partial t} \int \vec{u} dV + \oint \vec{u}(\vec{u} \cdot \hat{n}) dS = - \oint p\vec{n} dS + \frac{1}{\mathrm{Re}} \oint \nabla \vec{u} \cdot \hat{n} dS \tag{2}$$

where $\vec{u}$ is non-dimensional velocity vector, p is pressure, St is the Strouhal number, a non-dimensional frequency parameter given by $St = \omega L / U_o$ and $\mathrm{Re} = U_o L / \nu$ is the Reynolds number. ω is the imposed frequency, *L* the length scale, U_o the velocity scale and ν the kinematic viscosity. In the above equations subscript *v* denotes integration over the control-volume and ***n*** is a unit vector normal the face of the control volume. The above equations are to be solved with $\vec{u}(\vec{x},t) = \vec{u}_\partial(\vec{x},t)$ on the boundary of the flow domain where $\vec{u}_\partial(\vec{x},t)$ is the prescribed boundary velocity, including that at the immersed boundary. A second-order accurate, two-step fractional step method solution is advanced from time level *n* to *n+1* through an intermediate advection-diffusion step where the momentum equations without the pressure gradient terms are first advanced in time. A second-order Adams-Bashforth scheme is employed for the convective terms and the diffusion terms are discretized using an implicit Crank-Nicolson scheme. This eliminates the viscous stability constraint which can be quite severe in simulation of viscous flows.

2.3 Moving Immersed Boundaries

In the present work the immersed boundaries have prescribed motions. Therefore, the boundary conditions to be imposed on the solid-fluid boundaries are the no-slip and no-penetration conditions. The immersed boundary forms one side of the reconfigured boundary cells. Therefore, at that cell face the boundary conditions are specified. Depending on the location and local orientation of the immersed boundary, cells through which the interface passes typically assume trapezoidal shapes [3]. The key issue in the finite volume formulation is to evaluate convective and diffusive fluxes and pressure gradients on the cell-faces of these trapezoidal cells such that global second-order accuracy of the solver will be preserved. Since the procedures for constructing a consistent mosaic of control volumes in the vicinity of the interface yield arbitrary-shaped volumes, flux conservation needs to be enforced at contiguous cell faces of such cells. Furthermore, the current Cartesian grid method has been developed for unsteady viscous flows at moderately high Reynolds numbers. In such flows we expect that relatively thin boundary layers will be generated in the vicinity of the immersed boundary. These boundary layers are not only regions of high gradients but are often the most important features of the flow field. Thus, accurate discretization of the equations is especially important in the boundary layers. Since all the interfacial cells lie within the boundary layer, this is another reason why adequate local accuracy is desirable for these cells. In Ye et al.[3] we adopted a compact two-dimensional polynomial interpolating function which allows us to obtain a second-order accurate approximation of the fluxes and gradients on the faces of the trapezoidal boundary cells from available neighboring cell-center values. This interpolation scheme coupled with the finite-volume formulation guarantees that the accuracy and conservation property of the underlying algorithm is retained even in the presence of arbitrary-shaped immersed boundaries. This has been demonstrated in Ye et al.[3] for stationary immersed boundaries.

3 SIMULATION RESULTS

The test case chosen here to demonstrate the potential of this methodology for simulating fluidic micro-handling processes involves the settling of trapezoidal shaped blocks in a fluid under the influence of gravity. A closeup view of the block and substrate is shown in Figure 2. This configuration is intended to mimic the general process of fluidic assembly [4] wherein the substrate with the receptor sites would be situated on the bottom wall and the expectation is that in each pass, the blocks would settle down in the fluid and fill up the receptor sites. However, in order for a trapezoidal block to fill a receptor site it has to have the correct orientation.

The orientation of blocks settling in a fluid is governed by the stability of the body to moments generated by the pressure and shear stresses on the body. Thus the orientation of the block will depend on the block shape as well as flow parameters such as fluid density and viscosity. Thus, *a-priori*, it is difficult to know if a given combination of block shape and fluid will result in the desirable orientation. This is precisely where computational modeling of such processes can be useful since it provides a means of predicting the detailed features of the transport process.

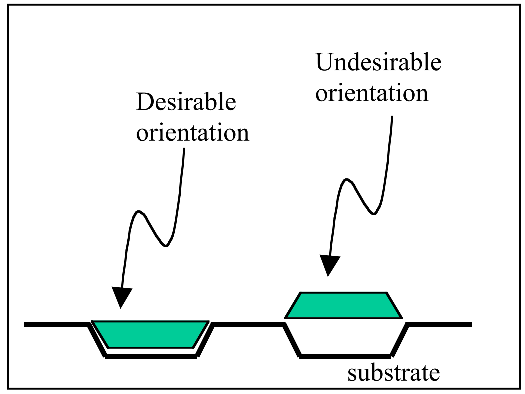

Figure 2. Schematic of block and substrate.

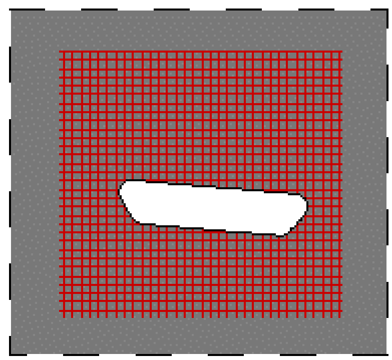

Figure 3. Shape of block and grid employed in the simulations.

In the current simulation, the motion of five blocks is simulated simultaneously in order to clearly demonstrate the ability of the method to handle multiple moving blocks. Figure 3 shows the geometry of one of the blocks and the underlying Cartesian grid. The primary objective here is to use the simulation to predict the preferred orientation of the blocks as they settle in the fluid. In order to accomplish this, a different initial orientation is chosen for each block and the initial orientation is shown in Figure 4a. The simulation is then initiated and the blocks allowed to settle under the influence of gravity. The simulations are carried out on DEC Alpha workstation and employ a uniform 550×500 Cartesian grid.

Figure 4b shows the orientation of the blocks at an intermediate time where the blocks have floated down to the middle of the domain and figure 3c shows the final situation where once of the blocks touches the bottom surface at which time the simulation is terminated. Interesting the simulation shows that despite the different initial orientation most of the blocks orient themselves in the desirable orientation as they settle in the fluid. Analysis of simulation results show that the trapezoidal shape of the blocks tends to set up a surface pressure distribution that always rotates the body into the desired orientation. Clearly, a different shape of the block might produce an entirely different outcome. Thus, the results clearly demonstrate the utility of the current method for simulating fluidic micro-handling processes and future work will involve further application of this methodology to problems in this arena.

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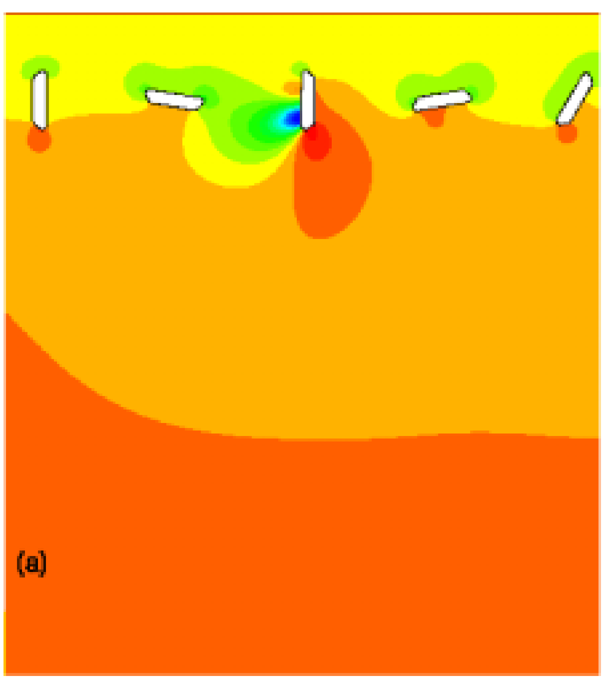

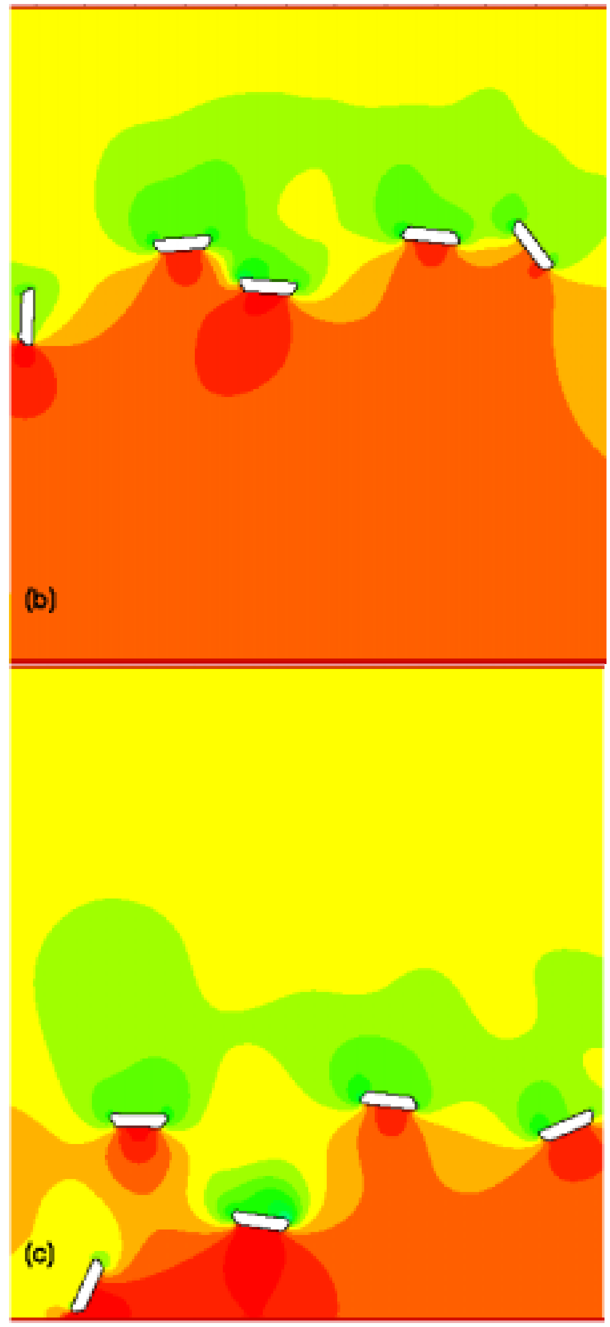

Figure 4. Results of simulations showing the settling of five blocks in fluid (a) Initial stage (b) intermediate stage (c) final stage