

Three Dimensional Simulations of Coating Flows: Methods for Large Free Surface Deformations and Moving Three-Phase Lines

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Abstract

Computational fluid mechanics techniques for examining free surface problems for coating flows in two dimensions is now a well-established procedure, owing much to the efforts of Scriven and his researchers.[1,2] Extending these methods to three dimensions requires a reconsideration of some of the same long-standing difficult issues for coating flows as well as special algorithms designed for the added geometric complexity. This paper presents a non-linear elastic pseudo-solid approach for deforming meshes in three dimensions. Special boundary conditions on the pseudo-solid mesh motion constrain its motion in the normal direction according to the relevant fluid physics, but allow shear-free motion of the mesh tangential to bounding surfaces. Within the standard Galerkin Finite Element formulation of the problem, these goals are achieved by locally rotating the pseudo-solid momentum vector equations at the boundaries. Moving or static contact lines provide a challenge in 3D because contact angle conditions must be imposed so that the fictitious solid, in which the mesh is embedded, may slide tangentially along three-phase lines unhindered. The computational techniques discussed in this talk are illustrated with two applications: solid-body rotation of fluid, and extrusion of an incompressible Newtonian fluid from a square nozzle.

Introduction

Prediction of the fluid mechanics of coating flows presents a special challenge to computational techniques because the position of the various material surfaces of the flowing liquid as well as the fluid velocity and pressure are unknown a priori. An attractive approach involves determining the shape of the computational domain simultaneously with the fluid flow. There are many methods for solving free and moving boundary problems, but this paper focuses on an approach which uses the finite element method (FEM) and incorporates a 'Full-Newton' iteration on both the Navier-Stokes equations and the moving mesh equations. By full Newton, we mean that all the equations are solved simultaneously and are assumed to be fully coupled.[3] This implies that the Newton-Rhapson iteration on the set of nonlinear algebraic equations resulting from the finite element formulation includes a Jacobian matrix which incorporates contributions from all the equations, and the order of the Jacobian matrix is almost twice that of comparable fixed boundary problems, with many additional nonzero entries accounting for the pervasive sensitivity of the equations to boundary deformations. The power of such a method has been demonstrated repeatedly for a wide variety of free-surface flow problems.[1,2,4]

In the past such methods have been applied primarily to two-dimensional and axisymmetric fluid flow problems. In some cases with geometrically simple flow domains these methods have been applied to three-dimensional flow problems [e.g. 5,6], but these applications have been limited to structured grids, decoupled methods, or small deformations. This paper displays initial three-dimensional results which demonstrate the applicability of the Full-Newton approach for complicated geometries and large free-surface deformations. The algorithms outlined here were implemented and tested in GOMA, a computational fluid mechanics code from Sandia National Laboratories.[7] This paper demonstrates the challenges of this method and how they are overcome while transforming from 2D to 3D.

Issues in Extending 2D Free-Surface CFD Methods to 3D

There are many steps involved in extending free surface computational fluid mechanics from 2D to 3D, and in this paper we discuss several of the most significant hurdles. The fully-coupled implementation of FEM leads to poorly conditioned matrix problems, which demands solution by direct methods; however, the work required to solve the 3D matrix problem directly grows precipitously with the size of the problem, mainly due to the increase in matrix band-width. Thus 3D demands a transition to iterative solvers. The other major hurdle deals with techniques for moving the mesh: the mesh deformation must be robust under large dilation and rotation, and the mesh must conform to the boundaries. To make a pseudo-solid mesh conform to the boundaries, the mesh equations are rotated near arbitrarily oriented surfaces.

Pressure Stabilization and Iterative Solvers

Difficulty arises in numerical solution of incompressible flow problems with the finite element method (FEM) due to the idiosyncratic nature of the mass balance when the fluid is incompressible. The mass balance, or continuity equation, for incompressible flow becomes an expression that the velocity is solenoidal and involves no other variables than the velocity. However, the mass balance equation is used to represent the behavior of the pressure, though the pressure is not explicitly included within it. Thus, when the problem is reduced to a matrix equation with the matrix containing the equations at each FEM node, zeros appear on the diagonal since the pressure equation contains no pressure variable. This makes inversion of the matrix quite difficult and robust direct solvers must be used. The problem with direct solvers is that they are both computational and memory intensive and hence ill suited for 3D flow problems.

The Galerkin least squares method, or pressure stabilization as it is also known, is used to stabilize the pressure equation by adding a nonzero term on the diagonal.[8,9] The standard finite element formulation weights the momentum equation and the continuity equation with the shape function used to describe the interpolation of the variables. When pressure stabilization is used, the momentum equation is dotted into the gradient of the Galerkin weight and added on to the Galerkin continuity equation weighted residual. This gives us a pressure term in the pressure equation, resulting in a non-zero diagonal and a modified continuity residual. The assumption here is that as the solution converges, the momentum residual will go to zero resulting in a truly solenoidal velocity field.

Once the Jacobian matrix has nonzero diagonal elements, the matrix equation become much easier to solve and iterative matrix solution techniques, such as GMRES and CGS, can be used that require much fewer computational resources and enable the solution of 3D incompressible flow problems. An added benefit to iterative solution techniques is that these algorithms parallelize efficiently, allowing solution on parallel architectures capable of solving much larger problems.

Pseudo-Solid Mesh Motion

Among the computational approaches available for free and moving boundary problems, the best choice depends on the particular problem. Each computational technique offers its own balance between efficiency, accuracy, and robustness [1,2,3,4] The most accurate techniques parameterize the free or moving boundary as a mathematical curve (two dimensions) or surface (three dimensions) in space, i.e., boundary parameterization techniques, so that boundary conditions may be applied precisely at an interface with a well-represented location, orientation and curvature. Moreover, exact boundary parameterization makes possible the solution of distinctly different field equations according to the governing physics in each region of the computational domain.

The purpose of this research is to make a boundary-conforming domain mapping technique as robust as possible. Here the term robust implies a technique that will most often succeed in converging to the solution, if a solution exists. Domain mapping techniques are distinguished from boundary mapping techniques; in the latter case the primary focus is on parameterizing the shape of an unknown free boundary with one less dimension than the computational domain. The focus of this work is to solve mesh-position equations simultaneously with the field equations which place no restriction on mesh structure and are amenable to the full-Newton approach. One such set of mesh-positioning equations meeting these guidelines for domain mapping are those describing the quasi-static deformation of an elastic solid continuum under boundary loads [3]. This pseudo-solid domain mapping procedure is suitable for a range of free boundary problems where the topology of the initial guess domain and the final domain are similar. The essential restriction is that the connectivity of the domain remain the same; e.g., a simply-connected domain is not permitted to evolve into a doubly-connected domain. A further requirement on the mesh motion is that it be robust under large deformations and rotations (as shown later in the paper). We use a large-strain Neo-Hookean constitutive equation to relate the pseudosolid stresses to the mesh strain.[7,10]

So-called distinguishing conditions serve to constrain the position or motion of the boundaries of the general deforming domain. These constraints, applied to the pseudo-solid deformation, differ from boundary conditions that are conventionally applied to solid materials in that they are not expressed specifically in terms of the mesh displacement or tractions, but rather in terms of whatever variables are relevant to the free boundary problem. Thus, the position of the fictitious solid on the interior of the domain is not coupled to the solution of the fluid mechanics problem. This coupling only occurs at the boundaries of the domain and is governed by distinguishing conditions. The mesh is boundary-fitting; i.e. the mesh must expand or contract so that it exactly fills the domain of the fluid. Thus the motion of the mesh is constrained in the direction normal to its boundaries, and slides in all tangential directions to relieve internal stresses of the fictitious solid.

Rotation of Mesh and Momentum Equations at Boundaries

At the boundaries, distinguishing conditions constrain the motion of the mesh in the normal direction; an issue is how to apply these conditions within the finite element framework. Because the mesh motion equations are vectorial, three mesh motion equations are associated with each nodal point. In simple situations the choice which of the three mesh momentum equations to replace by the boundary condition is easy because the surface lines up with a coordinate plane (i.e. if the surface were a plane facing in the y direction, the plane boundary condition would replace the y component of the mesh momentum equation). Such simple rules break down in general cases, especially when the boundaries rotate during the computation. Note that replacing a normal-directed momentum equation by a distinguishing condition not only constrains the normal motion of the boundary but also implies (through the weak formulation of the finite element method) mesh is stress-free in the remaining two tangential directions. Note too, that ad hoc procedures for choosing different natural coordinates based on the instantaneous surface orientation can lose continuous differentiability and therefore lose the quadratic convergence of Newton's Method. Choosing the wrong mesh equation to replace by a distinguishing condition causes mesh distortions near the boundary that resemble tangential shear stresses along the boundary. In general the best looking meshes result when the mesh is tangentially shear free near the boundary.

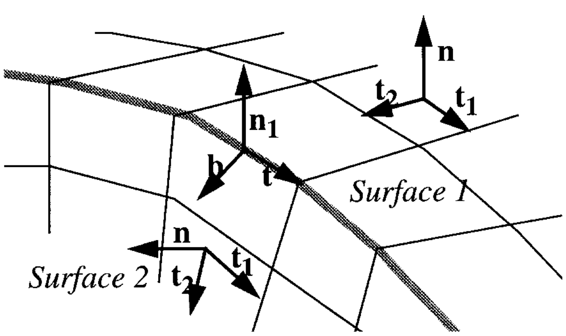

Figure 1: Illustration of the issues surrounding rotation of mesh equations on surfaces and edges.

Thus we choose to rotate all of the mesh equations along the boundary into normal-tangential form and replace the normal component of the rotated equations by the distinguishing condition [3]. This method has proven effective in 2D to produce meshes which undergo a large degree of rotation and deformation [7,11]. An additional problem occurs in 3D, however, which is especially evident when using unstructured grids: the normal-tangential rotation of the equations is not unique because all tangents in the plane of the surface are equally valid. Thus for efficient numerical computation, the tangents in 3D must be chosen using a protocol that is independent of which element or node is currently active and that is independent of the orientation of the surface. We have tried a variety of methods; the two most successful methods to obtain the first tangent vector use seed tangents and basis vectors. The second tangent vector is obtained by a cross product between the normal and the first tangent vector.

Seed tangents can be used to force a tangent to orient in a consistently reproducible direction by projecting the tangent onto the plane, $\boldsymbol{t}_1 = (\boldsymbol{I}\text{-}\boldsymbol{nn})\bullet\, \boldsymbol{s}.\boldsymbol{t}_1$ is the first tangent vector in the plane, $\boldsymbol{I}$ is the identity matrix, $\boldsymbol{n}$ is the unit vector normal to the plane, and S is the seed vector, this sector must be normalized to obtain a unit vector. This meth-od works well for nearly flat surfaces and breaks down when the seed vector is nearly coincident with the normal vector.

The local element basis vectors can also be used as tangent vectors. This method only works if the tangent resulting from one element is then used to seed the calculation of the tangent in an adjacent element (strictly, this methods is performed on a node-by-node basis to ensure that each node feels the weighting of all adjacent elements). As shown in the results section, this method enables efficient rotation of the mesh to any angle.

At an edge where two surfaces intersect, the line tangent (along the curve of intersection), $\boldsymbol{t}$, is well defined except for its direction. To determine the direction of the tangent, one of the intersecting surfaces is labeled as the primary surface whose normal is labeled $\boldsymbol{n}_1$, and the cross product between $\boldsymbol{n}_1$ and the line tangent is defined as the binormal, $\boldsymbol{b}$, which is defined as outward pointing from the primary surface, this determines the direction of the line tangent in a consistent and reproducible fashion

Sample Results

These methods have been applied to several applications [11]. Here we present two applications, one which demonstrates the accuracy of the results for fluid under solid-body rotation and another which demonstrates the power of the method for analyzing a more complex extrusion problem.

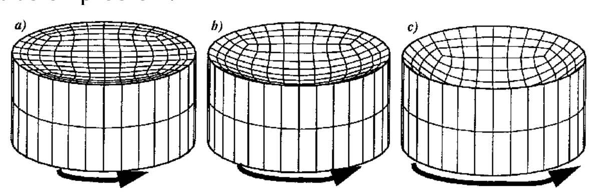

Figure 2. Sample predictions of 3D free surfaces of a fluid under solid-body rotation with angular velocities that cause vertical displacements of a) Δz = 0,05 b) Δz = 0.25 c) Δz = 0.5.

Solid-Body Rotation of Fluid with a Free Surface

The free surface of a fluid in solid body rotation becomes a paraboloid of revolution (in absence of surface tension) at steady-state. Thus this is a simple problem for testing whether the 3D fluid mechanics computations are producing the correct results. Figure 2 displays predictions for a fluid in a rotating cup. The mesh is unstructured and obeys the kinematic condition that serves as the distinguishing condition of the material surface. There is no-slip between the fluid and the walls or bottom of the cup, so there. The contact line where the free surface meets the cup wall is pinned at a fixed position and the angle is not constrained. Using a fixed contact line simplifies the edge conditions and alleviates the need for a constraint on the volume, which is implied by the constraint on the height of the contact line. As the angular velocity of the cup, ω, increases the free surface sags further into the cup:

$$\Delta z(0) = \frac{\omega^2}{2g} \quad (1)$$

$\Delta z(0)$ is the depth that the free surface sags at the axis of rotation, and g is the magnitude of gravity; this result is independent of density and viscosity.

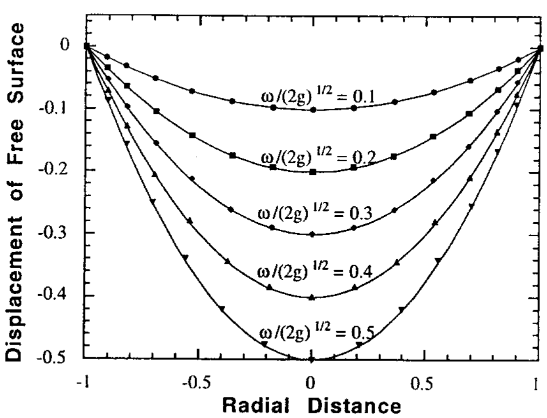

Figure 3. Comparison between free surface shape predicted by 3D Computational Fluid Mechanics (symbols) and the analytical result (lines) for a fluid in solid-body rotation.

Figure 3 shows the comparison between the results of this model and the standard analytical solution for a range of angular velocities. For all the results shown the finite element predictions match the analytical results. Note that a match between our results and the analytical solution is not trivial because the finite element mesh does not possess cylindrical symmetry.

Extrusion from a Square Nozzle

Many industrial processes involve extrusion of a liquid from an orifice; the subsequent evolution of the fluid cross section is of interest. This example problem displays predictions of fluid exiting from a nozzle of square cross-section and falling under gravity (Figure 4). The fluid enters the nozzle under an applied pressure force and has zero velocity (no-slip) along the walls of the nozzle. The free surface is pinned to the lip of the nozzle. The fluid exits the domain with an assumed zero shear and tangential stresses that approximates the physical situation; strictly, the fluid stream accelerates under the action of gravity and continues to thin, ultimately breaking up. The conditions chosen for the results in Figure 4 ensure that the shape of the jet is sensitive to the competing effects of gravity, inertia, capillary forces, and viscosity. Using the nozzle half-width and the maximum velocity at the nozzle entrance, the Reynolds number is about 12.5, the Capillary number 1.7, and the Froude number 10.

These solutions were predicted using continuation starting from a nozzle oriented vertically (labeled in Figure 4). During initial solution of the problem, the free surface evolved from a square to a nearly circular cross-section through the combined actions of surface tension and viscosity. Then the nozzle was slowly rotated (in increments) to achieve the results in Figure 4. Several problems arise in this problem when the nozzle rotation becomes large: 1) the mesh at the nozzle exit becomes distorted, 2) the elements at the bottom of the mesh elongate in order to reduce dilational and shear stresses, and 3) some oscillations in the free surface occur as the mesh distortion becomes too large. Increasing the discretization (currently 8600 unknowns) should help alleviate some of these problems.

Conclusions

This paper demonstrates a method for solving 3D free-surface fluid mechanics problems using a boundary fitted mesh and fully-coupled nonlinear Newton's method. The primary conclusion is that such a method does work, and produces solutions that match analytical results in simple cases, and match intuition in more difficult cases. We expect to be applying this method to a wide variety of manufacturing processes in the near future.[11]

Acknowledgments

This work was performed under a contract from Sandia National Laboratories which is supported by the United States Department of Energy under contract DE-AC-4-76-DP85000.

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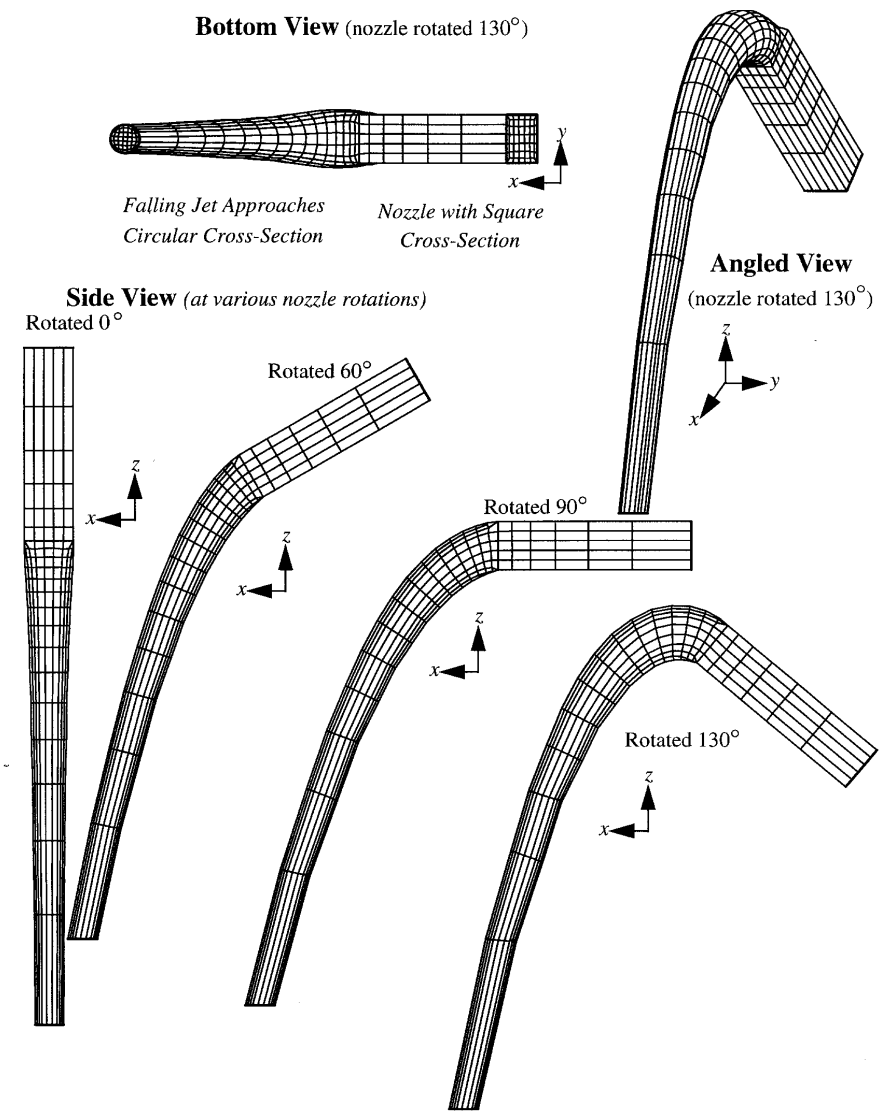

Figure 4. Sample predictions of fluid extruding from a nozzle of square cross-section and bending under gravity. ρ *= 1 gf/cm*^{3}*,* μ*=1 poise,* σ*=30 dynes/cm, g = 980 cm*^{2}*/s,* w_{nozzle} *= 0.5 cm, Re = 12.5, Fr = 10.2, Ca = 1.7,*$v_{max,nozzle}$ *= 50 cm/s.*

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11. To see a display of other results using these techniques see our web-page (http://www.me.udel.edu/~cairncro/goma/home.html)