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subject: **SLIDE COATING** Templates and tutorial for GOMA (GT-011.2)

keywords: slide coating, multilayer coating, free surface flow strategies, trouble shooting for free surface flows, remeshing

input records: GD_LINEAR, GD_PARAB, SURFTANG, KINEMATIC

Introduction

This tutorial assumes the user has gone through the beginner's training tutorial on GOMA and SEAMS (GT-001.4). Specifically, it assumes the user has a strong familiarity with GOMA itself and the tools `fastq`, `ex1ex2v2`, `aprepro` and `blot`. If not, please go through that tutorial if you have it, or contact Duane Labreche (dalabre@sandia.gov) or Randy Schunk (prschun@sandia.gov) to get it.

This tutorial addresses multilayer slide coating, specifically three miscible layers coated simultaneously. It can be simplified quite readily to one- or two-layer slide coating by setting the properties of each layer to be the same. In fact, the first revision of this tutorial makes the assumption that all layers possess the same thermophysical properties with only the flow rate in each layer allowed to be different. The missing link to achieving the generalized case, with each layer possessing unique properties, hinges on a numerical or analytical solution to stratified flow of multiple layers of liquid flowing down an inclined plane surface. Closed form solutions are rarely tractable for more than two layers, especially for non-Newtonian viscosities. This template makes it clear where and how the numerical or analytical solution of the velocity field upstream at the inflow plane is to be incorporated in the model. The mechanism will involve "include" files and a table-lookup boundary condition.

The key to running all of these problems is to obtain a good initial guess and then to know the details of the problem parameterization. This tutorial will try to cover all phases. The template itself, if you choose not to generate a solution for your specific problem, uses parameters similar to those in the Ph.D. thesis of Kostas Christodoulou ("The Fluid Mechanics of Slide Coating", Ph. D. Thesis, University of Minnesota, 1989; available from University Microfilms, Ann Arbor, MI). Those parameters can be varied within a fairly narrow range before the mesh becomes too distorted. This tutorial should be combined with the remeshing capability covered in

document GT-006.3 for a more general solution, or at least to redesign the mesh once a solution has been found. It is very difficult to grid-up an initial geometry with mesh features that will follow, in a robust way, all free surface motion.

Three-Layer Slide Coater

The files discussed in this tutorial which comprise the slide coating template are in a directory called `slide_template/free_lower` and are available from Duane Labreche. The files critical to this template are `3layer_inp.fixed`, `3layer_inp.1free`, `3layer_inp.2free`, `3layer_inp.3free`, and `3layer_inp.4free`. These are a hierarchical set of *GOMA* input files designed to guide you from an initial fixed grid solution to the complete solution with four free surfaces (a bottom meniscus, a top meniscus, and two immiscible interfaces). The geometry file (`fastq` input file) which embodies the overall geometry and thermophysical parameters is called `geometry3`, and is included in the same directory. The material files are somewhat trivial, corresponding to Newtonian liquids with constant properties, so they will not be discussed here.

Figure 1 illustrates the basic geometrical features and parameterization of the three-layer model. In slide coating, liquid issues from a narrow feed slot through the slot die, and then joins other layers from other feed slots until they reach a fully-developed, stratified flow on the inclined plane surface. This model does not take into account the flow rearrangement around the feed slots. The basic assumption is that the flow is fully developed on the slide at the inflow plane. As discussed below we require a prescribed velocity profile at either the inflow or outflow. In this tutorial we experiment with such conditions on both inflow and outflow, depending on the situation. The velocity profile on the slide depends on the flow rate of each layer, the rheological properties of each layer, the density of each layer, and the slide angle relative to gravity. Only in the unrealistic case that all layers have the same properties and each layer is Newtonian is a velocity profile analytically tractable from the governing equations. That is the case we take up here, but with clear instructions on how to generalize. When the flow encounters the moving web at the base of the slide, it must bridge a narrow gap and thus expose a second external surface, herein referred to as the *lower meniscus*. The web then rapidly entrains the film, starting at a dynamic contact line, or here referred to as the *DCL*, into the final coated film. The flow domain is cut off on the upper left where the film becomes fully developed. There the velocity profile is that of a plug flow, with a slight correction due to gravity (i.e., a Nusselt profile). Other features that are noteworthy are the static contact line, or *SCL*, where the lower layer (layer1) separates from the slide; the slide face which is the inclined surface over which the liquid flows down; and the die lip, under which the lower layer wets.

What makes this problem challenging are the numerous (four total in the three-layer case) free surfaces that must be released, parameterized and tracked. This tutorial takes you through one step-by-step strategy of obtaining a solution for this problem, but surely other strategies exist. The fact that the flow and free surfaces start in one

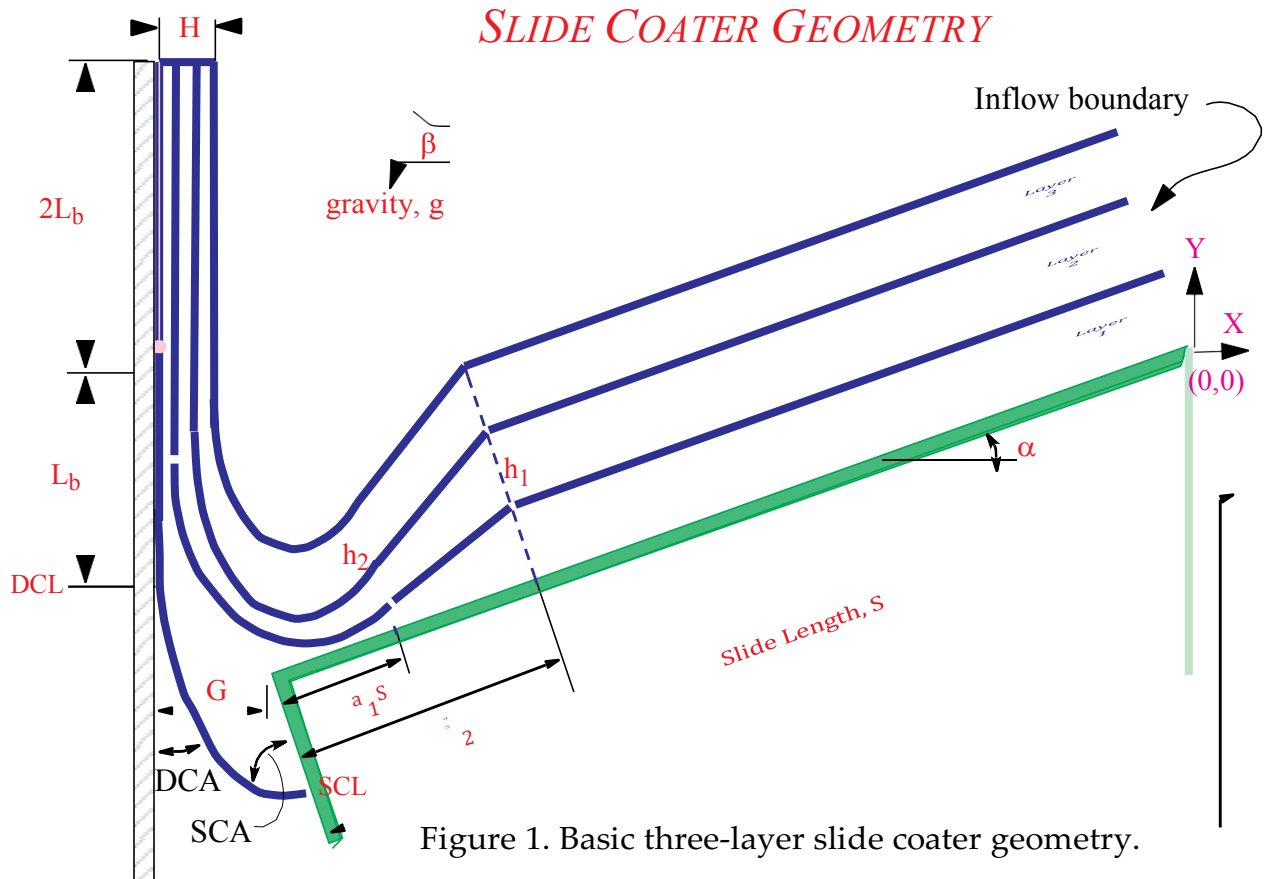


Figure 1. Basic three-layer slide coater geometry.

orientation and direction and end in another at the outflow with no confining walls on the top makes for large scale mesh motion, and further complicates the problem.

The mesh as generated with `fastq` from the file `geometry3` is shown in Figure 2. It is basically structured in most regions, with the exception of the bead or bridge region where the flow impinges on the moving web. The first part of this discussion addresses the geometry and parameter-specification file `geometry3`. The top part of that file looks like:

```

$ Thermo-Physical Properties (all units cgs)
$ degrees-to-radians {DTR = PI/180.}
$
$ viscosity {visc1 = 0.1}
$ {visc2 = 0.1}
$ {visc3 = 0.1}
$ density {dens1 = 1.0}
$ {dens2 = 1.0}
$ {dens3 = 1.0}
    
```

Distribution

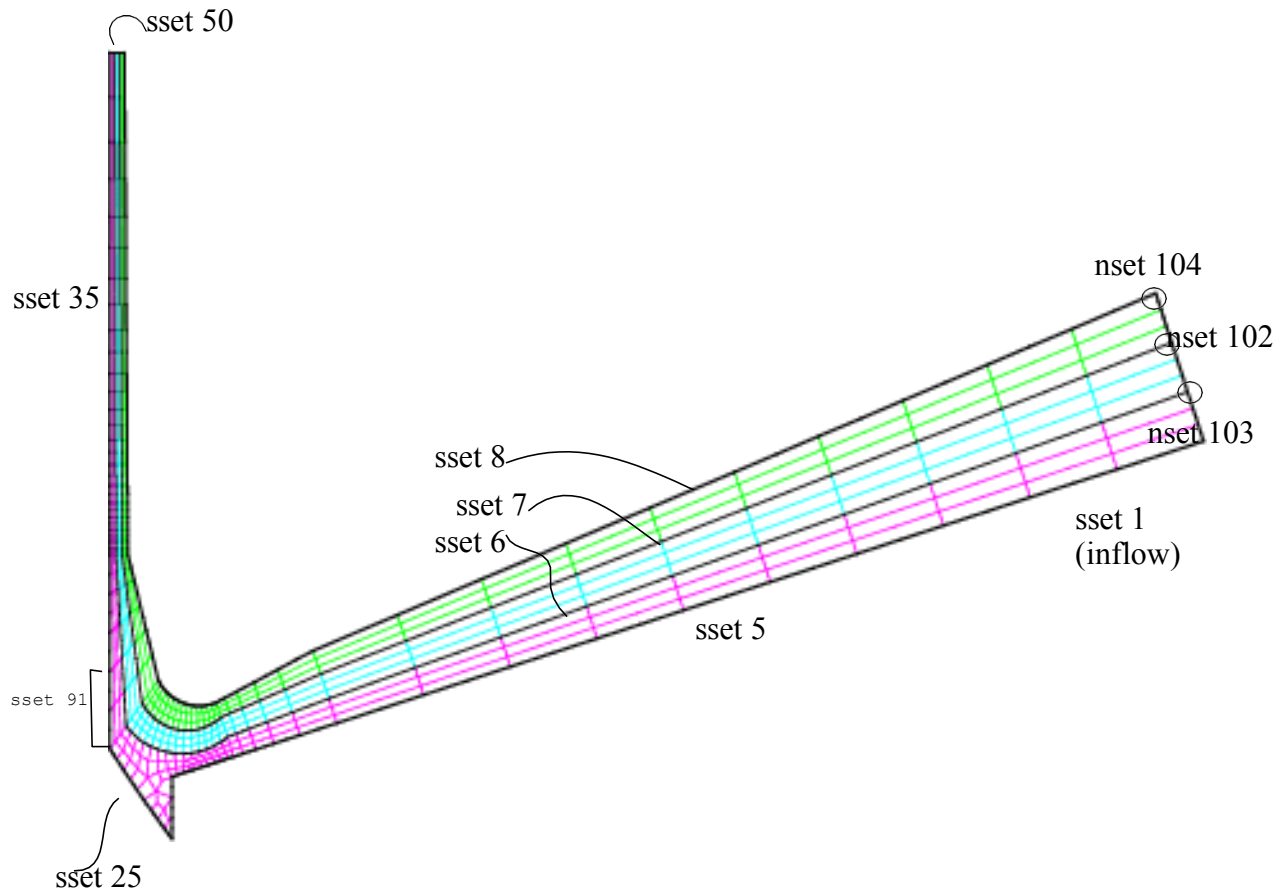


Figure 2. Initial finite element mesh for three-layer wetted die face case.

```

$ surface tension      {st1  = 70.0}
$                      {st2  = 70.0}
$ {st3  = 30.0}
$ gravity              {grav  = 980.}
$
$ static contact angle          {SCA1 = 30.}    {scar1 = SCA1*DTR}
$ dynamic contact angle        {DCA1 = 50.}    {dcar1 = DCA1*DTR}
$
$ dynamic contact angle (ref.)  {dcar0 = 140*DTR}
$
$ OPERATING CONDITIONS
$ final thickness layer 1      {ft1  = 0.003}
$ final thickness layer 2      {ft2  = 0.003}
$ final thickness layer 3      {ft3  = 0.003}
$ webspeed                   {websp = 100.}    {websp_new = 100.}
$ flowrate layer 1             {q1   = websp*ft1}
$ flowrate layer 2             {q2   = websp*ft2}
$ flowrate layer 3             {q3   = websp*ft3}
$ slide angle with horizontal {alpha = PI/10.}  {alpha_new = PI/10.}
$ angle of gravity vector      {beta  = 0.}
$
$ CALCULATION OF FILM THICKNESSES
$ (NB! DENSITIES AND VISC OF BOTH LAYERS ARE THE SAME FOR NOW!)

```

```

$
$ {cosab = cos(PI/2-alpha+beta)}
$ {denom = dens1*grav*abs(cosab)/viscl}
$ {q = (q1+q2+q3)/denom}

$ OK HERE is where you put your complicated formulas for figuring the
$ inlet film thickness of each layer, given the specified final
$ thicknesses desired. Here we assumed all layers have the same
$ props and that the final film thicknesses are such that the initial
$ thickness of each layer is the same. We can do better. Actually,
$ The ft1, ft2, vars for the final thicknesses set above are just
initial
$ guesses. With what I have here, those thickness at the outflow will
$ be quite different. With this specification, the bottom layer will
$ be the thinnest in the outflow. We need now to import the results
$ of a 1D inclined plane flow code, which gives us the initial
$ thickness of each layer given the initial flowrates. Those numbers
$ will be imported here via an include file as the initial velocity
$ profile in goma via a BC_TABLE boundary condition.
$
$ The example here shows that the thickness of each layer can be
changed,
$ thereby changing that layers flowrate.
$
$ {tsl1 = (3*q)**(1./3.)/3} {tsl1_new = 1.7*(3*q)**(1./3.)/3}
$ {tsl2 = tsl1} {tsl2_new = tsl1}
$ {tsl3 = tsl1} {tsl3_new = tsl1}
$

$ Thin out initial guess a little more
$
$ film thickness factor (h2/h1) {b1 = 0.4}
$ film thickness factor (h3/h1) {b2 = 0.30}
$ web film thickness {Hoo = (ft1+ft2+ft3)}
$ slide film thickness {h1 = tsl1+tsl2+tsl3}
$ slide thickness in transition {h2 = b1*h1}
$ slide thickness in transition {h3 = b2*h1}
$ slide length {S = 7.0*h1}
$ slide transition factor 1 {a1 = 0.06}
$ slide transition factor 2 {a2 = 0.2*0.8}
$ bead length {Lb = 1.48721*Hoo*Hoo*dens1*webssp/viscl}
$ web length from top of slide {W = 1.0*h1}
$ coating nip (die face and web) {G = 0.4*h1} {G_new = 0.4*h1}
$ drag zone length factor {dzf = 1.0}
$ drag zone length on die face {Ld = dzf*G}
$ die face angle from vertical (ccw+) {gamma = 0.}

$Parameters for Geometry of Lower Meniscus (layer 1)
$tangents of contact angles {tanSCA = tan(PI/2-scar1)}
$ {tanDCA = tan(dcar1-PI/2)}
$tangent ratio {TR = (tanSCA+tanDCA)/tanSCA}
$ epsilon for the problem {eps = ft1}

$Parameters for Bead Region

```

Distribution

```

$shape factor for upper bead layer 1      {shape1 = 0.30}
$shape factor for upper bead layer 2      {shape2 = 0.30}
$shape factor for upper bead layer 3      {shape3 = 0.30}
$90% mean velocity of web                 {mv90 = 0.90}
$80% mean velocity of web                 {mv80 = 0.80}
$50% mean velocity of web                 {mv50 = 0.50}
$tangent(60 degrees)                      {tan60=tan(60*DTR) }
$tangent(45 degrees)                      {tan45=tan(55*DTR) }

```

\$

This file is responsible for all geometrical and physical property input through extensive use of **APREPRO**. The file itself is included in the *GOMA* input files (discussed below) and the material files for each layer. The relevant properties of each layer are entered first, for the simple Newtonian case. Notice that now all layers are taken as the same material, so tracking interfaces between them amounts to tracking a streamline in the flow. Another important property of the problem is the static contact angle (see Figure 1) as specified here to be 30 degrees (converted to radians with the **DTR** variable defined at top). A parameter that is also important is the dynamic contact angle, here specified to be 50 degrees.

The operating parameters of the flow are input next, starting with the desired final film thickness of each layer, **ft1**, **ft2**, and **ft3**. Together with the web speed, viz. **websp**, we can calculate the volumetric flow rate per unit width for each layer, or **q1**, **q2** and **q3**. So, given the slide angle **alpha** and the angle of the web relative to the gravity vector **beta**, the film thickness on the slide can be computed for this simple case, as is done next (viz. **ts11**, **ts12**, and **ts13**). Here we are currently making a major assumption regarding the thickness of the layers at the inflow, given their flow rates. We have specified the outflow film thicknesses and hence flow rates of each layer to be equal in this example. This clearly means that the inflow film thicknesses will not be the same, and in fact should lead to a thinnest layer at the top and the thickest at the bottom due to the Poiseuille flow profile. Here we are assuming they are the same. The upshot of this is that in the final solution the final layer thicknesses will adjust accordingly, i.e., the thinnest layer will be on the bottom. Note the extensive comment section of what needs to be done to make this problem complete. Basically we need to have the inflow layer thicknesses and velocity profiles to be input to the problem, as derived from an external source. This can be done with a simple include file in the **geometry3** file, and a **GD_TABLE** boundary condition in the *GOMA* input file. *This exercise is left up to those who use this template for production.* The remaining parameters are used to help specify the shape of the initial geometry. The reader can use **fastq** and Figure 1 to study the effect of these. Many parameters require care when adjusting, as they dictate the smoothness of the assumed free surface positions.

All of these parameters can be adjusted before the problem is started. In some cases the operating parameters affect the geometry, as is the case for the final layer thicknesses and the webspeed which together determine the inflow film thickness. In any case, be careful adjusting these parameters. In fact, as it is currently set up much improvement to the free surface portions of the geometry are needed. Ideally, smooth spline-like

curves would provide the easiest means of finding a solution. **Smoothness between the sections is critical. Kinks in the surface make convergence slow, and in many cases, impossible.** If you adjust the initial guess to the surface shape, do it in such a way as to keep the surfaces smooth.

By way of review, recall from previous tutorials that *GOMA* solves for displacements of the nodes, not the absolute coordinates. The only positions in the model that are pinned are the intersections of the inflow plane with the top surface and internal interfaces (3 points), and occasionally the static and dynamic contact line during startup. So, any parameter affecting these points can only be adjusted after a solution has been found in a way that keeps track of the displacements. Note that there are five such adjustable geometric parameters: the slide angle `alpha`, the coating nip `G`, and the inflow film thickness `ts11`, `ts12` and `ts13`. Note that the lines specifying these parameters require you to define the original value (i.e., the value which is used for the original mesh) and the new value, e.g. `alpha_new`. Below we will change a few of these and observe the effect.

The rest of the file `geometry3` is basically the `fastq` geometry commands. There is extensive use of `APREPRO` to figure out the points and lines of this geometry.

The most complicated portion of the problem formulation is the boundary conditions. In fact, it is the only portion of the *GOMA* input deck we will discuss here. All other settings regarding solvers, file input redirection and problem description (for 3 layers, `layer1.mat`, `layer2.mat` and `layer3.mat`) are similar to those of slot coating and roll coating and are discussed elsewhere (see training documents on beginners/GT-001.4, slot/GT-002.1, roll/GT-003.1). We will discuss the boundary conditions while referring to specific portions of the domain.

We begin with the inflow portion, which is explained in Figure 3 where the boundary conditions on problem geometry (mesh motion equations) and fluid mechanics (momentum equations) are given. On the slide and inflow planes we have the usual `PLANE` boundary conditions on mesh motion. These are given on the lower right of the figure. Notice how the slide angle `alpha` is needed for the calculation of the coefficients of the slide plane. The inflow plane coefficients are computed with simple algebra using the coordinates of points 1 and 2. Point 1 is at the intersection of these two planes and it is the origin of the problem [0,0]. Points 2, 3 and 4 are given the single-node node set IDs of 102, 103 and 104 respectively, as shown in the figure. These points denote the intersection of each layer interface with the inflow plane, and their positions are also computed based on `alpha`. So when the slide angle `alpha` is changed AFTER a solution has been found, we clearly see by these conditions that the inflow plane and slide plane are rotated about the origin (Point 1). Notice how the `alpha_new` variable is used in the boundary conditions. It is also used to compute `[x2,y2]`, `[x3,y3]` and `[x4,y4]` in file `geometry3` which is included in the *GOMA* input file for use here. The boundary conditions on `dx` and `dy` on node sets 102, 103, 104 reflect the resultant displacement change due to an angle change. It is very important to note the optional float 1.0 that appears after each `dx` and `dy` condition. This tells *GOMA* to apply these dirichlet

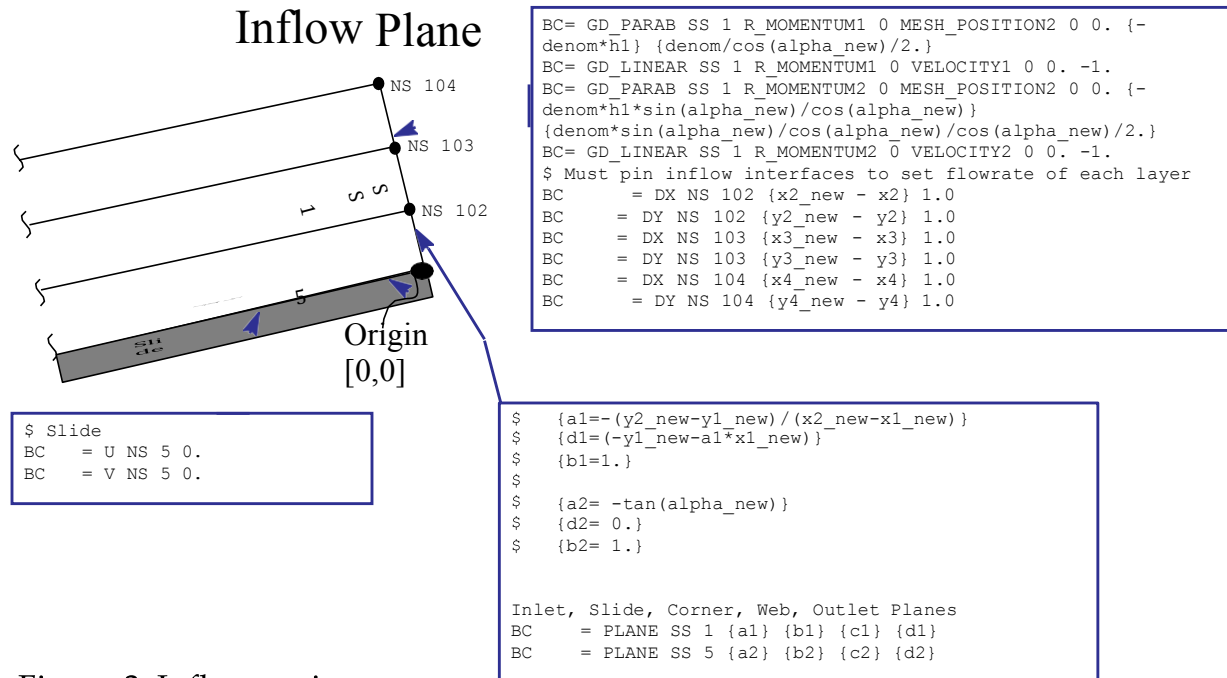


Figure 3. Inflow region

conditions in a residual form, and not in a “hard-set” form, so that these points are iterated slowly to the new rotated state. Consult the *GOMA* manual for more details on this.

As for the velocity field in the inflow region, we have no-slip applied to the slide surface (nset 5), and a prescribed velocity profile prescribed on the inflow using a complicated combination of the GD_ conditions. As an exercise, convince yourself that those four GD_ conditions apply the following inflow velocity profile:

$$u = -\text{denom} \cdot h1 \cdot y + [\text{denom} / \cos(\alpha)] / 2 \cdot y^2$$

$$v = -[\text{denom} \cdot h1 \cdot \sin(\alpha) / \cos(\alpha)] \cdot y + [\text{denom} \cdot \sin(\alpha) / \cos(\alpha)^2 / 2] \cdot y^2$$

where

$$\text{denom} = \text{dens1} \cdot \text{grav} \cdot \text{abs}(\cos \alpha) / \text{visc1}$$

$$h1 = \text{tsl1} + \text{tsl2} + \text{tsl3} \text{ (total slide layer thickness)}$$

It is here where we need to furbish this template to allow for generalized inflow velocity component data. This data will come from an independent source, like a one-dimensional code that can compute the layer thickness and resultant profile for Newtonian and nonNewtonian liquid layers with varying properties. The **GD_TABLE** condition will then supplant this assumed parabolic profile which is based on all three layers having the same physical properties.

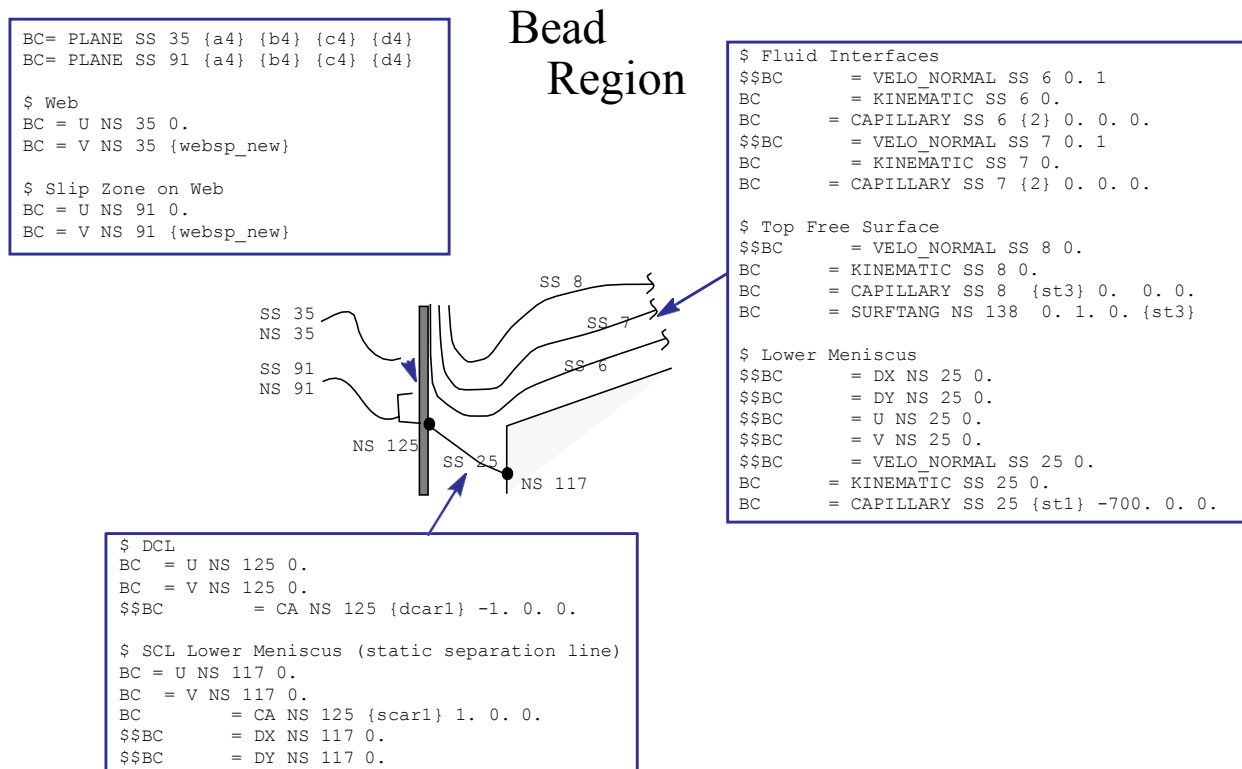


Figure 4. Free surfaces and bead region.

Figure 4 illustrates the boundary and interfacial conditions in the “heart” of the flow around the coating bead. Here we show solid-wall geometry conditions as well as free surface conditions. The only user-prescribed geometry in this region corresponds to the web and the slide lip. The web is made up of PLANE commands for side set 35 and side set 91, which are colinear. Side set 91 is a presupposed slip region over which the Navier-Slip condition can be applied. In the case shown here, both regions are given a velocity field corresponding to the webspeed, which implies no slip over the entire web. Some slip is applied at the dynamic wetting line and over the first element in this case by virtue of setting the velocity at the DCL (nset 125) to zero in order to satisfy the kinematic paradox. Note also there, and across the lower meniscus (side set 25) we set dynamic and static contact angles with the **CA** boundary condition.

The surfaces that are free to move according to the conservation of mass, or as material surfaces in this case, are the lower meniscus (side set 25), the top free surface (side set 8) and the two interfacial boundaries (side sets 6 and 7). Notice how at the internal interfaces we have a very small surface tension. It turns out that zeroing the surface tension works fine. These are miscible layers and so no surface tension is appropriate. In this particular case, because all the layers possess the same properties, these surfaces correspond to stream lines in the flow. Corresponding to the top free surface we have the usual **CAPILLARY** and **KINEMATIC** cards, and the corresponding extra “integrated by parts” term with the **SURFTANG** card at the intersection with the outflow

plane. On the bottom meniscus, note the applied back pressure of 700 dyne/cm². This specification was determined as a part of the solution process.

The only remaining portion of the domain to discuss is the outflow region. This region is not pictured here. It corresponds to side set 50, as shown in Figure 2. There we specify the geometry with a **PLANE** command and the velocity profile to be fully-developed with a **VELO_TANGENT** card. There is one exception to this, as will be discussed in the startup procedure below.

Solution Startup Procedure

As we mentioned earlier, the startup procedure presented here is not unique. It worked for this case. The description here is intended to give you some experience for flows of this nature.

The solution procedure begins with generating a mesh, viz.

```
fastq -a -m slide.gen geometry3
ex1ex2v2 slide.gen slide.exoII
```

As usual we need to obtain a smooth “fixed grid” solution that will serve as an initial guess to our free surface solutions. In the template directory there are five GOMA input files:

```
3layer.inp.fixed          3layer.inp.3free
3layer.inp.1free         3layer.inp.4free
3layer.inp.2free
```

Run in sequence, with zeroth-order continuation, these files represent a path to the final solution at the given parameter set. Using the Unix **diff** command between each one in succession will give you an idea of what was added in each step. We feel it is important though to guide you through the steps and present the critical concepts.

IMPORTANT FREE SURFACE INFORMATION HERE:

The first step generates a flow field on fixed but “shear free” interfaces and surfaces. Actually, it applies **VELO_NORMAL** boundary conditions to the top and interfacial surfaces, and zero velocity to the bottom free surface with **u** and **v** BCs. Finally, you will notice that the **GD_** type boundary conditions on the inflow velocity profile have been commented out, and a boundary condition of the following form

```
$ Outlet
BC      = VELO_TANGENT SS 50 0 0. 0. 0.
BC      = VELO_NORMAL SS 50 {webssp}
```

applied to the outflow. The reason for this is that this is the only way we could produce a smooth velocity profile along the free surfaces using the **VELO_NORMAL** command, which

-11-March 17, 1999

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gives pathological results when the free surface “guess” is not perfectly smooth. When you generate a fixed grid solution for any free surface flow, look carefully at the velocity field with blot, especially on critical junctions of the presupposed free surface. Often times, if the surface is “kinked” there, the **VELO_NORMAL** boundary condition will lead to artificial recirculations and a noisy field. Your convergence on the free surface case (i.e., when **KINEMATIC** is substituted for **VELO_NORMAL**) is doomed if such noise exists. In order for us to get rid of the noise in this problem, we had to make our top free surface as smooth as possible and change the inflow/outflow conditions appropriately. This is just experience, but it applies to all free surface flows. Ultimately, with higher-order curve representations in more modern mesh generators like **PATRAN** and **CUBIT**, we should be able to avoid these problems in the future, but the only way to circumvent them with **fastq** is to play with the intersections of lines and circular arcs until you get smoothness.

Also note that we choose a peculiar “zero-velocity” condition for the lower meniscus. We will relax this on subsequent steps, but using **VELO_NORMAL** there on the first step also leads to peculiar noise in the fixed grid solution. The only other place we have seen this phenomenon is in our roll coating templates.

END OF IMPORTANT FREE SURFACE INFORMATION

So the fixed grid solution is obtained by

```
goma -a -i 3layer.inp.fixed
cp soln.dat contin.dat
```

The next step is to release the top surface, which is the hardest. Nonetheless, the sequence queued up in the **run1** script provided works.

```
source run1
cp soln.dat contin.dat
```

or follow the relaxation path in that script, viz.

```
goma -a -i 3layer.inp.1free -r 0.01 -n 20
cp out.exoII out.exoII.tmp
cp soln.dat contin.dat.1
cp soln.dat contin.dat
goma -a -i 3layer.inp.1free -r 0.05 -n 10
cp soln.dat contin.dat
goma -a -i 3layer.inp.1free -r 0.1 -n 20
cp soln.dat contin.dat
goma -a -i 3layer.inp.1free -r 1.0
cp soln.dat contin.dat
```

Here you will see a remarkable change in the surface shape, and appreciate how poor our initial guess was. In the future, with some experience, we would redesign the mesh at this point to include some of the features of the solution.

Distribution

The next step releases the interface corresponding to side set 7. The input file for this is `3layer.inp.2free`. You can run the “run2” script or follow the sequence below:

```
#
goma -a -i 3layer.inp.2free -r 0.0071 -n 30
cp -f out.exoII out.exoII.tmp
cp -f soln.dat contin.dat.1
cp -f soln.dat contin.dat
goma -a -i 3layer.inp.2free -r 0.05 -n 25
cp -f soln.dat contin.dat
goma -a -i 3layer.inp.2free -r 0.1 -n 10
cp -f soln.dat contin.dat
goma -a -i 3layer.inp.2free -r 1.0
cp soln.dat contin.dat
```

The next step releases the second interface between layers 1 and 2 and allow for a more realistic velocity field on the lower meniscus, with the contact lines and lower meniscus still fixed in position (N.B. the `dx` and `dy` boundary conditions on node set 25). Notice how we remove the velocity boundary conditions on node set 25 (bottom meniscus) which set the velocity to zero there, and apply the `KINEMATIC`, `CAPILLARY` and `CA` cards even though it is still fixed. You can run the “run3” script for this step, which is

```
#
goma -a -i 3layer.inp.3free -r 0.0071 -n 30
cp out.exoII out.exoII.tmp
cp soln.dat contin.dat.1
cp soln.dat contin.dat
goma -a -i 3layer.inp.3free -r 0.05 -n 25
cp soln.dat contin.dat
goma -a -i 3layer.inp.3free -r 0.1 -n 10
cp soln.dat contin.dat
goma -a -i 3layer.inp.3free -r 1.0
```

Now, with that solution saved you can release the lower meniscus. As with the slot coating tutorial, we first look at the solution with `plot` and pick off the pressure which would be required to keep the meniscus fixed in position. We find that -700 dyn/cm^2 will suffice. Notice how also we apply the contact angles on the DCL and SCL on this final step. The following sequence in the “run4” script gets the final solution:

```
goma -a -i 3layer.inp.3free -r 0.05 -n 25
cp -f soln.dat contin.dat
goma -a -i 3layer.inp.3free -r 0.1 -n 10
cp -f soln.dat contin.dat
goma -a -i 3layer.inp.3free -r 1.0
cp soln.dat contin.dat
```

A few sample results are shown below.

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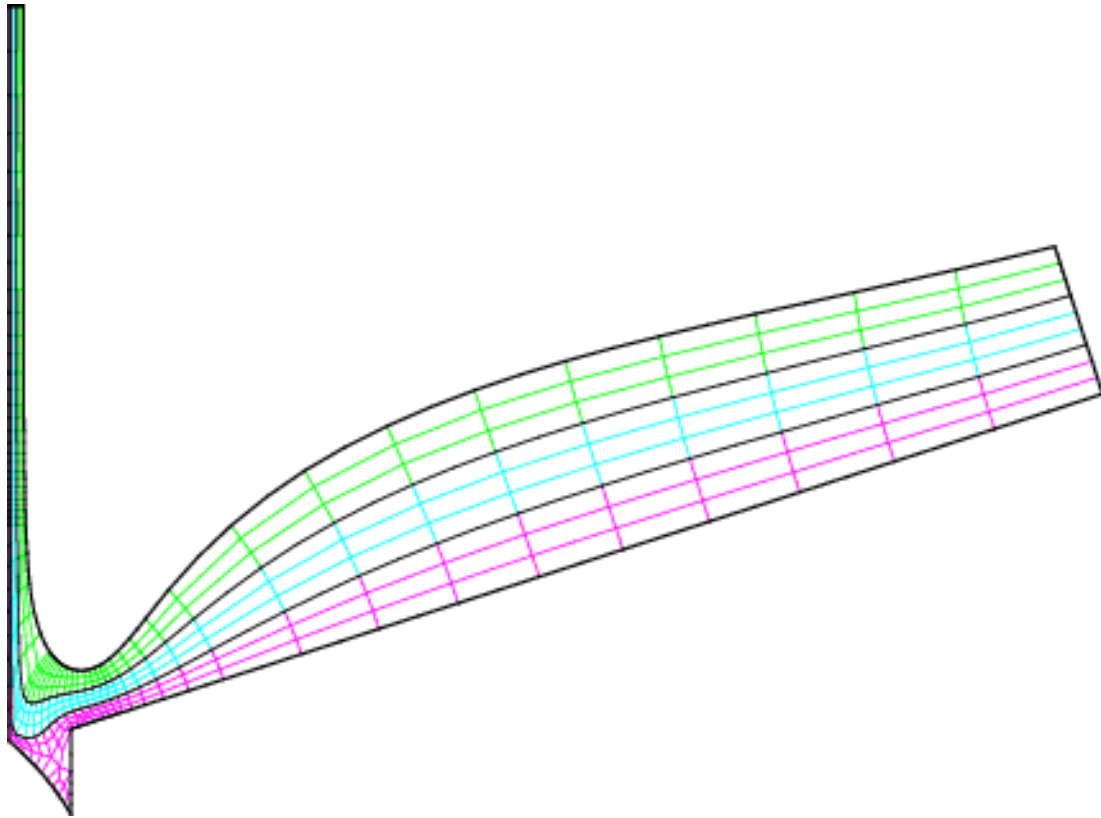


Figure 5. Base case solution. (Deformed mesh)

In the first figure (Figure 5) we show the base-case solution. In the next figure (Figure 6) we show the result of increasing the slide angle by a few degrees. In the last figure (Figure 7) is the result of increasing the flow rate of the lower layer by 10%. Note the much larger bead region, which attests to the sensitivity of the solution.

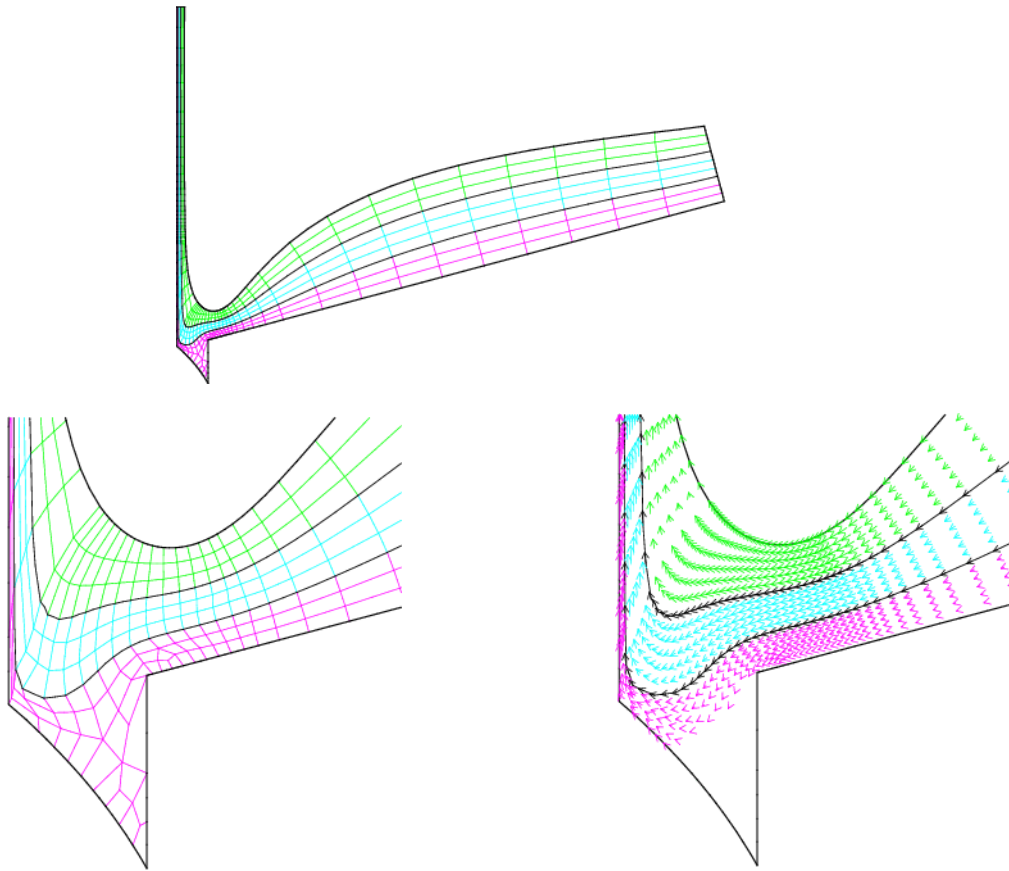


Figure 6. Solution with a 5% increase in slide angle alpha, over the base case.

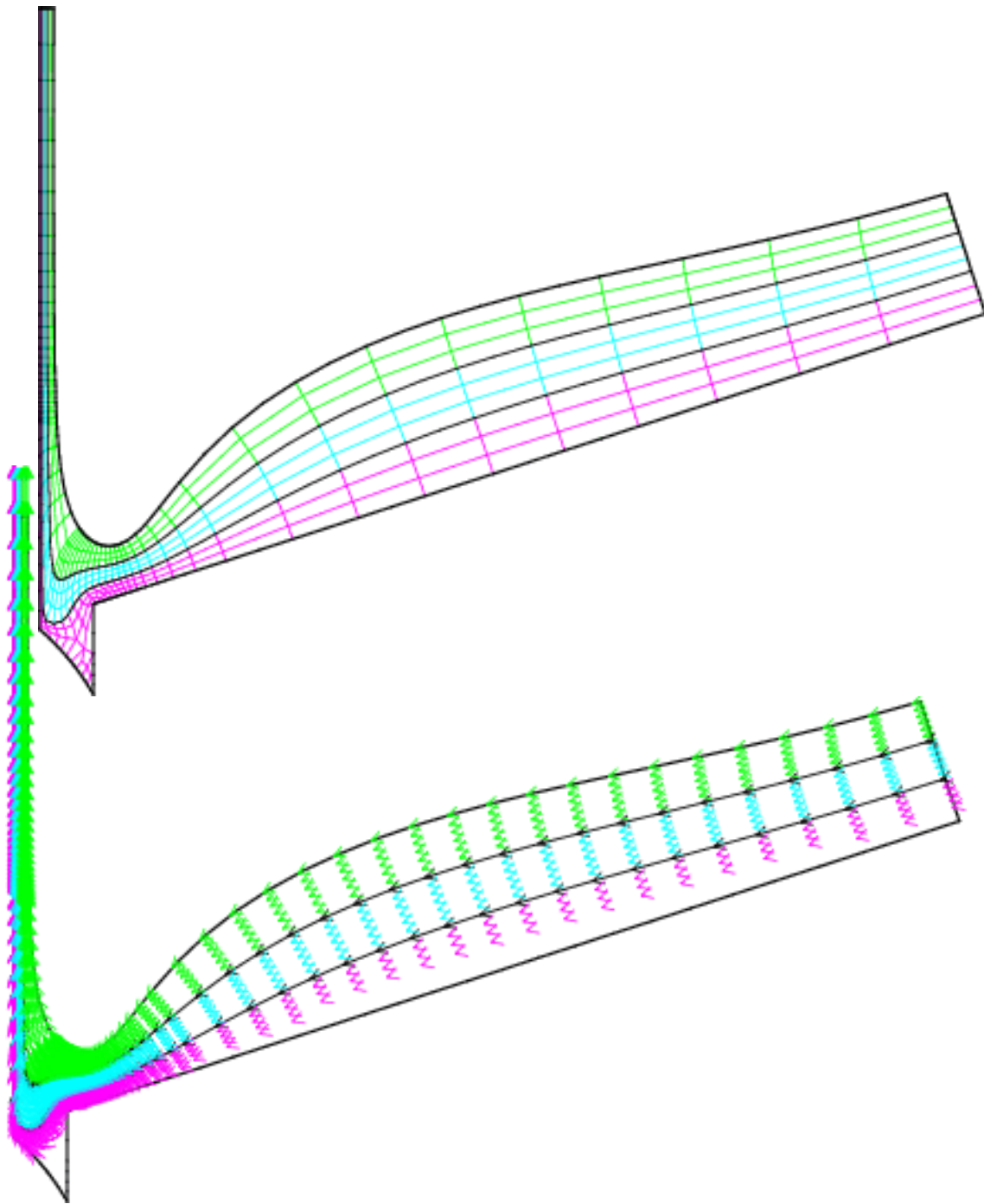


Figure 7. Solution with a 10% increase in the flowrate of the bottom layer.