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subject: Tutorial on droplet on incline problem (GT-007.2)

keywords: three dimensional, rotation boundary conditions, drops

input records: ROT, VELO_SLIP, VELO_NORMAL_EDGE, VELO_TANGENT_EDGE, VAR_CA_EDGE, ROT=MOM,
ROT=MESH, BASIS, BASIS=RESEED, BASIS=FIRST

Introduction

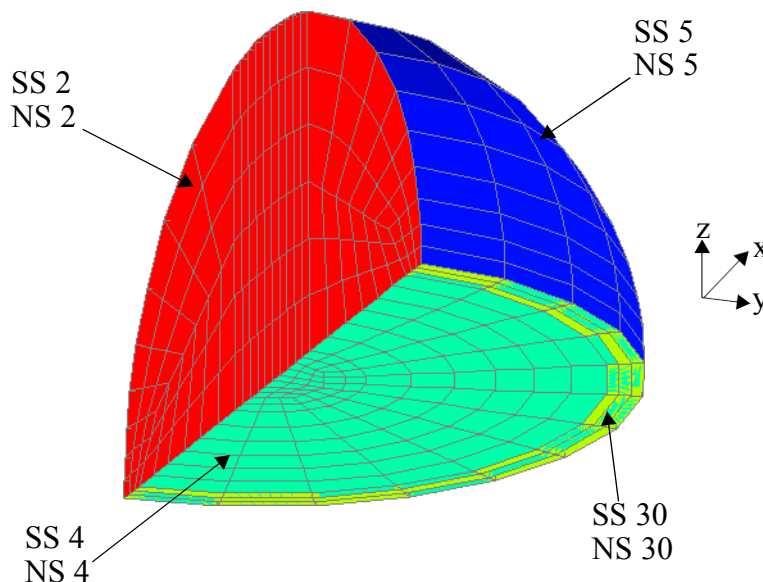
The motion of a droplet down an inclined plane is one of the simpler problems involving a three dimensional dynamic contact line. Therefore, it is ideal for illustrating how to employ the capabilities that exist in GOMA in solving problems of this class. A short description of the mesh and its boundary side sets and node sets will be followed by a lengthy discussion of the input deck. In particular, emphasis will be placed on the ROT conditions and the contact line boundary conditions. Finally, some results will be shown.

Mesh and Boundary Sets

The droplet mesh is shown in Figure 1. It is in fact only half of the actual droplet. The inclination of the substrate surface will be in the direction of the x axis, hence the $y = 0$ plane is a plane of symmetry. Solving only half of the problem, of course, has advantages in reducing the number of unknowns needed, but also the presence of the symmetry plane in the problem provides a measure of determinacy to the mesh equations. Without it, rotary modes of mesh motion could appear.

Figure 1 also shows the side sets and node sets used. Side set 5 encompasses the curved free surface. Node set 2 is the plane of symmetry ($y = 0$). The underside of the drop in contact with the inclined substrate is decomposed in a slightly more complicated manner. Side set 4 includes the entire surface in contact with the substrate. However, there is an additional side set, side set 30, that extends over just the three bands of narrow elements adjacent to the contact line. Node set 30 coincides with side set 30. Finally, node set 4 is composed of the nodes on the underside excluding the nodes in node set 30, that is, the interior nodes. The reason for this choice of boundary sets on the underside will become apparent shortly.

Figure 1. Droplet mesh, node sets and side sets.



Input File

The input file, *droplet.input*, is shown below:

```

FEM File Specifications
---
FEM file                = droplet.exoII
Output EXODUS II file   = out.exoII
GUESS file               = contin.dat
SOLN file                = soln.dat
Write intermediate results = no
Anneal Mesh on Output   = yes
---
General Specifications
---
Number of processors     = 1
Output Level            = 0
Debug                   = 0
Initial Guess           = zero

Time Integration Specifications
---
Time integration         = transient
delta_t                 = -0.00025
Maximum number of time steps = 100
Maximum time            = 2.0

```

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```

Minimum time step      = 1.e-9
Maximum time step     = 0.001
Time step parameter   = 0.
Time step error       = 1.0 1 1 0 0 1 0
Printing Frequency    = 1
Initial Time          = 0.0

```

Solver Specifications

```

---
Solution Algorithm    = gmres
Preconditioner       = ilu
Size of Krylov subspace = 100
Orthogonalization    = modified
Maximum Linear Solve Iterations = 200
Number of Newton Iterations = 12
Newton correction factor = 1
Normalized Residual Tolerance = 1e-8
Residual Ratio Tolerance = 1e-5
Pressure Stabilization = yes
Pressure Stabilization Scaling = 0.01

```

Boundary Condition Specifications

```

---
Number of BC =      -1

# Free Surface
BC = CAPILLARY SS 5 1.0 0.0 0.0

BC = KINEMATIC SS 5 0.0

# Underside

BC = U NS 4 0.
BC = V NS 4 0.
BC = W NS 4 0.

BC = VELO_SLIP SS 30 0.01 0. 0. 0.

BC = W NS 30 0.0

BC = PLANE SS 4 0. 0.0 1. 0.0

# Symmetry Plane

BC = V NS 2 0.

BC = DY NS 2 0.

# Edge conditions

BC = VELO_NORMAL_EDGE SS 5 4 0.0
BC = VELO_TANGENT_EDGE SS 5 4 0.0 0.0 0.0
BC = VAR_CA_EDGE SS 5 4 90. 0.99 0. 0. 0.

```

END OF BC

Rotation Specifications =

ROT = MOM EDGE 4 5 VELO_NORMAL_EDGE 5 VELO_TANGENT_EDGE 5 W 30 NONE
 ROT = MOM VERTEX 4 5 2 VELO_NORMAL_EDGE 5 VELO_TANGENT_EDGE 5 W 30 NONE

ROT = MESH SURFACE 4 T1 0 T2 0 PLANE 4 SEED 1. 0. 0.
 ROT = MESH SURFACE 2 T1 0 DY 2 T2 0 SEED 1. 0. 0.
 ROT = MESH SURFACE 5 T1 0 KINEMATIC 5 T2 0 BASIS_RESEED

ROT = MESH EDGE 4 5 VAR_CA_EDGE 5 T 0 PLANE 4 NONE
 ROT = MESH EDGE 2 5 T 0 DY 2 KINEMATIC 5 NONE
 ROT = MESH EDGE 2 4 T 0 DY 2 PLANE 4 NONE

ROT = MESH VERTEX 2 4 5 VAR_CA_EDGE 5 DY 2 PLANE 4 NONE

END OF ROT

Problem Description

Number of Materials = 1

MAT = fluid 1

Coordinate System = CARTESIAN
 Element Mapping = isoparametric
 Mesh Motion = ARBITRARY
 Number of bulk species = 0

Number of EQ = 7

EQ = mesh1	Q1	D1	Q1	0	0	0	1	0	0
EQ = mesh2	Q1	D2	Q1	0	0	0	1	0	0
EQ = mesh3	Q1	D3	Q1	0	0	0	1	0	0
EQ = momentum1	Q1	U1	Q1	1	1	1	1	1	0
EQ = momentum2	Q1	U2	Q1	1	1	1	1	1	0
EQ = momentum3	Q1	U3	Q1	1	1	1	1	1	0
EQ = continuity	Q1	P	Q1	1				0	
				div	ms	adv	bnd	dif	src porous

In the FEM specifications section we see that the starting mesh configuration should be present in the file *droplet.exoII* when the problem is started. For subsequent restarts, the mesh information will be contained in the file *contin.exoII*. We note also that we have requested mesh annealing at the conclusion of each computation. This is a process where the coordinates of each node are updated with the current displacement values. The displacement fields are then zeroed, effectively removing the mesh stress (hence the term “annealing”). This is an important part of obtaining solutions because the translation of the droplet will result in larger and larger displacements as time progresses. Eventually, convergence of the iterative solver is affected by this and they must be removed with this annealing process.

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In the Time Specifications, we note that using the - sign in front of the time step size terms turns off the variable time step feature. Thus, the time step is fixed at -0.0025. This was done because of the problem with large displacements affecting iterative solver convergence. It was necessary to exert considerable control over how big the time step was and how many time steps were taken to effectively deal with this problem.

The GMRES iterative solver was chosen to solve the linear algebra problem for each iteration. The parameters listed in the Solver section were found to produce robust accurate results. Because we are using an iterative solver, pressure stabilization is also employed. The stabilization parameter shown above allowed for minimal intrusion of the PSPG terms into the accuracy of the solution yet allowed for robust convergence usually.

There are several things to note in the list of BCs. Note first, the VELO_SLIP card assigned to side set 30. This is a necessary feature for solving 3D dynamic contact line problems with GOMA. It allows for a region where the fluid velocity can relax from the values imposed by the contact line to the no slip conditions imposed on the rest of the fluid/substrate interface. Note that the impenetrability condition is enforced on side set 30 with a Dirichlet condition. The VELO_SLIP condition would also enforce this constraint but the Dirichlet condition makes it more explicit. Note also the Dirichlet conditions imposed on the mesh and velocity fields on the symmetry plane (SS/NS 2). These could be replaced by PLANE and VELO_NORMAL conditions, but these would add to the length of the ROT list. Finally, there are the three edge conditions, VELO_NORMAL_EDGE, VELO_TANGENT_EDGE, and VAR_CA_EDGE. The former two enforce the kinematic paradox in three dimensions, the latter sets the contact angle as a function of the local rate of advance or recession of the contact line with respect to the substrate. These conditions are essential to the solution of this problem. Note that for each, the free surface side set is specified first followed by the substrate side set. See the GOMA manual for more in depth descriptions of these conditions and the parameters associated with them. The PLANE SS 4 card is of course required to allow the mesh (not necessarily the fluid) to slip along this plane.

Because the computational domain is simple, the size of the ROT specifications section is not large. The VELO_NORMAL_EDGE and VELO_TANGENT_EDGE are both rotated conditions on the momentum equation, so ROT conditions are required on the edge where they are specified. The MOM_VERTEX card is included for completeness. Because the PLANE 4 and the KINEMATIC 5 conditions are also rotated conditions, MESH SURFACE rotation cards are needed. These cards identify what rotations of equations will be done and how these rotations will be organized. Consider the card associated with the PLANE 4 surface:

```
ROT = MESH SURFACE 4 T1 0 T2 0 PLANE 4 SEED 1. 0. 0.
```

This card indicates that on side set 4 the x, y, and z mesh equations will be rotated to give two components in two independent tangential directions and one component normal to the surface. The card indicates that the two tangential components (T1 0 and T2 0) will be retained, but the normal component will be replaced by the PLANE 4 constraint. The order that these appear is also important because it indicates which component or constraint will be associated with what degree of freedom on that surface. In this case, the card also indicates that in the global matrix the x displacement unknown is associated with the T1 component, the y unknown with the T2 component and the z unknown with the PLANE 4 constraint. In all ROT cards, this order is the same, first x then y then z.

In the case of MOM rotation specifications, the association is with the x, y and z velocity components.

If a direct solver is used on the linear algebra this association is not important. If an iterative solver is used, however, the association can be crucial. The essential rule is to associate a boundary condition with the coordinate it is most sensitive to. In this example, the PLANE 4 constraint constrains the nodes in side set 4 to the $z = 0$ plane. It is most sensitive, therefore, to the z coordinate. It is not sensitive at all to the x or y coordinate. Indeed, if the PLANE 4 constraint was placed in either the x or y place in the above card the result would likely be overflows or underflows. Of course, there are situations in which the constraint is sensitive to all three coordinates at once. In those cases, it is less clear cut what the appropriate association is and this usually has to be determined through trial and error.

The last part of each ROT card concerns identifying the appropriate seed vector. There are, of course, an infinite number of independent tangent basis vectors from which to choose. The user is required to identify this choice by specifying a seed vector option. In the above example, a fixed SEED vector is set: (1,0,0). This vector identified here is then projected into the surface at each point a tangent vector is needed. The unit vector in the direction of this projection is the first tangent vector (T1). This tangent vector is crossed with the surface normal vector to get the second tangent vector (T2). Thus, when using the SEED option in this card, it is very important to choose a vector that is never normal to any part of the surface in question. Of course, there are situations where the choice of a seed vector is problematic. Curved surfaces in particular often give rise to situations where it is very difficult to choose a seed vector that is not normal to at least one element. For these cases, there are other options for specifying seed vectors. One of them, BASIS_RESEED, is in fact used in the ROT condition for the KINEMATIC surface. Others are BASIS and BASIS_FIRST which are discussed in the Goma manual. In general, they use the local element edges to provide seed vectors for determining the tangents. BASIS_RESEED seems to be the most robust, although, trial and error is often the rule when employing these other seeding algorithms. Note that EDGE and VERTEX ROT conditions do not need a seed specification. Instead they use a vector along the edge itself as one basis of the rotation matrix, the vector normal to the first side set specified in the ROT command as the second basis, and the cross product of these two vectors, referred to as the binormal, as the third basis.

When specifying ROT conditions, the following rule should be kept in mind. If two surfaces share a node, the rotated BC's that will be applied to it are those identified with the ROT SURFACE card that occurs *first* in the file. However, if an EDGE card is specified for this node, the BC's identified on the EDGE card will be applied. Likewise, if there are two EDGE cards that could apply to a node, the EDGE card that occurs first in the file will be the one used. However, if a VERTEX card is included for this node, the VERTEX card's BCs will be applied. Thus, in summary, the order of ROT preferences is:

VERTEX -> *first* EDGE *in file* -> *first* SURFACE *in file*

Note, however, the Dirichlet conditions take precedence over all ROT specifications.

Material Property File

The material property file, *fluid.mat*, appears below:

```

${theta=30.0}
${gx = 980*sind(theta)}
${gz = 980*cosd(theta)}
${sig = 72.75}

---Physical Properties
Density= CONSTANT 1.

---Mechanical Properties and Constitutive Equations
Solid Constitutive Equation = NONLINEAR
Convective Lagrangian Velocity = NONE
Lame MU = CONSTANT 10.
Lame LAMBDA = CONSTANT 1.
Stress Free Solvent Vol Frac= CONSTANT0.
Liquid Constitutive Equation = NEWTONIAN
Viscosity= CONSTANT0.1
Polymer Constitutive Equation = NOPOLYMER

Surface Tension= CONSTANT{sig}

---Thermal Properties
Conductivity= CONSTANT1.
Heat Capacity= CONSTANT1.
Volume Expansion= CONSTANT1.
Reference Temperature= CONSTANT0.
Liquidus Temperature= CONSTANT1.
Solidus Temperature= CONSTANT1.

---Microstructure Properties
Media Type= CONTINUOUS
Porosity= CONSTANT0.0
Permeability= CONSTANT0.0

---Electrical Properties
Electrical Conductivity= CONSTANT0.

---Brinkman-equation parameters
Brinkman Porosity= CONSTANT0.0
Brinkman Permeability= CONSTANT0.0
FlowingLiquid Viscosity= CONSTANT0.0
Inertia Coefficient=CONSTANT0.

---Species Properties
Diffusion Constitutive Equation = FICKIAN
Diffusivity = CONSTANT 00.
Latent Heat Vaporization= CONSTANT 00.

```

```

Latent Heat Fusion= CONSTANT 00.
Vapor Pressure = CONSTANT 00.
Species Volume Expansion= CONSTANT 01.
Reference Concentration= CONSTANT 00.

*****Species Number*****|

----Source Terms
Navier-Stokes Source= CONSTANT {gx} 0. {-gz}
Solid Body Source= CONSTAN 0. 0. 0.
Mass Source= CONSTANT0.
Heat Source= CONSTANT0.
Species Source= CONSTANT 0 0.
Current Source= CONSTANT0.

```

The *.mat* file for this problem shown above is unremarkable. The only points to be noted are the Surface Tension card which sets it to a constant value. Because this card is present in the *.mat* file, the surface tension parameter appearing in the CAPILLARY BC card is treated as a multiplier on the value of surface tension entered in the *.mat* file. The incline is “tipped” by simply having a non-zero x-component of the Navier-Stokes source. Note how the *aprepro* preprocessor permits us to easily specify any tipping angle desired.

Solution procedure

The problem is started by invoking Goma from the command line

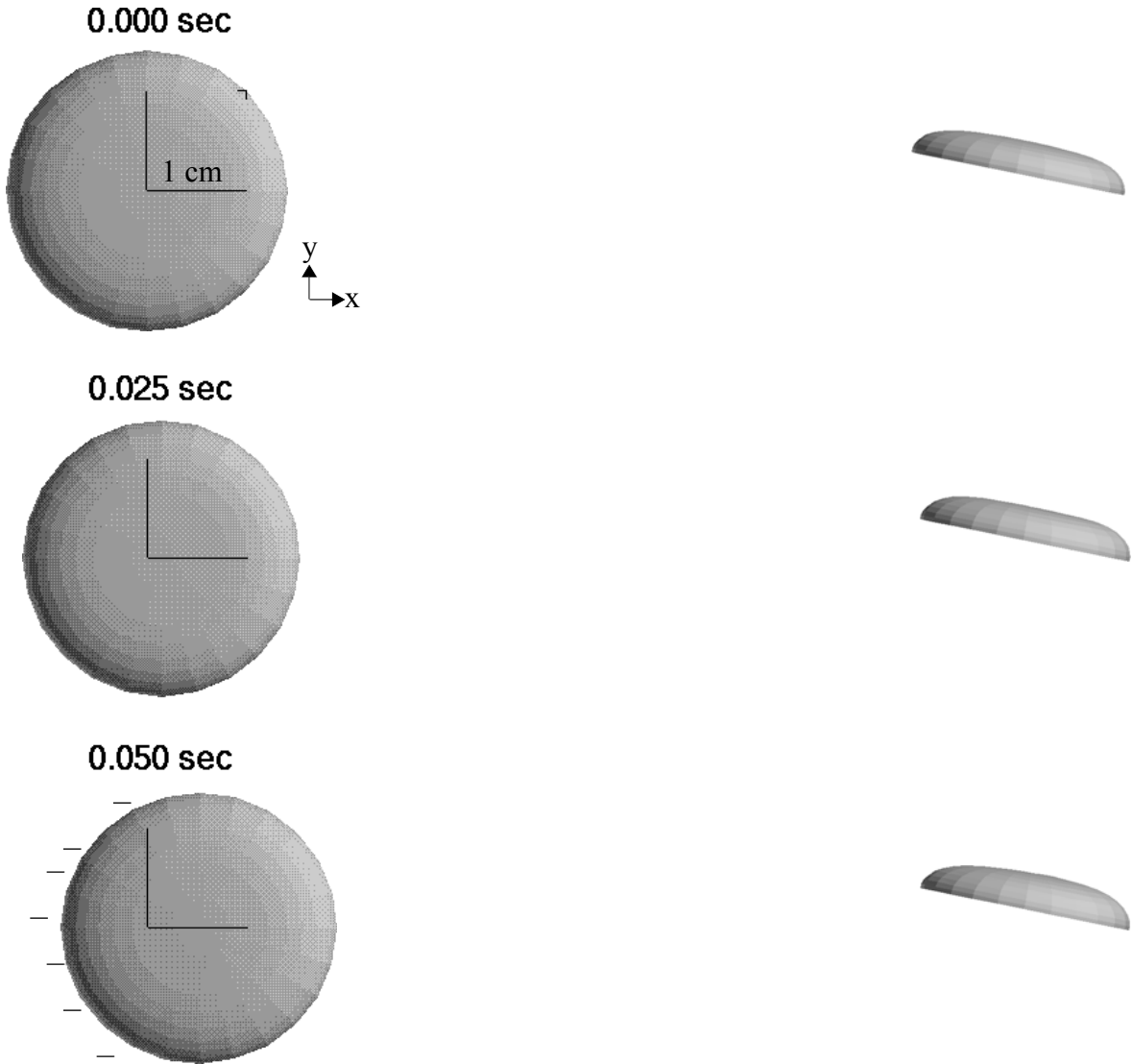
```
% goma -i droplet.inp -a
```

The time integration should proceed easily at first with convergence of the Newton-Raphson solver in five to six iterations and the iterative solver in less than 50 iterations. The displacement of the droplet down the incline will start to become so large, however, that the number of iterative solver iterations will gradually start to increase from time step to time step. Eventually, the iterative solver will no longer be able to provide accurate solution of the linear algebra problem and the Newton-Raphson iteration will fail as a result. All is not lost, however. The last accurate time plane should be copied into the *contin.exoII* file and the problem restarted with zero time steps set on the Number of Time Steps card. The resulting *anneal.exoII* file has the same velocity and pressure field as the last accurate time step, but the coordinates of the nodes have been altered in accord with the displacement fields and the latter have been set to zero. The next step is to copy the *anneal.exoII* file into the *contin.exoII* file, change the initial time value in the input file to the last time plane found, and restart the time integration. Eventually, the same difficulty will be encountered and the same procedure must be repeated. In fact, as the speed of the droplet increases the procedure will have to be repeated with greater frequency.

Results

Figure 2 shows a sequence of planform and side frame views of the droplet as it begins to accelerate down the incline. As time progresses, the shape of the droplet becomes more and more elongated in keeping with intuition and fluid tends to shift to the downhill side. Ultimately, a “rooster tail” appears

at the trailing edge. This is not thought to be physical but instead an indication of the mesh becoming poorly conformed in that area due to accumulated mesh deformation. Evidence for this is the inverted “V” shape that the trailing edge has become in the final frames. Remeshing of the domain at an intermediate point would be a remedy to this behavior. Alternatively, the original mesh could be reworked to concentrate more elements at the rear of the droplet.



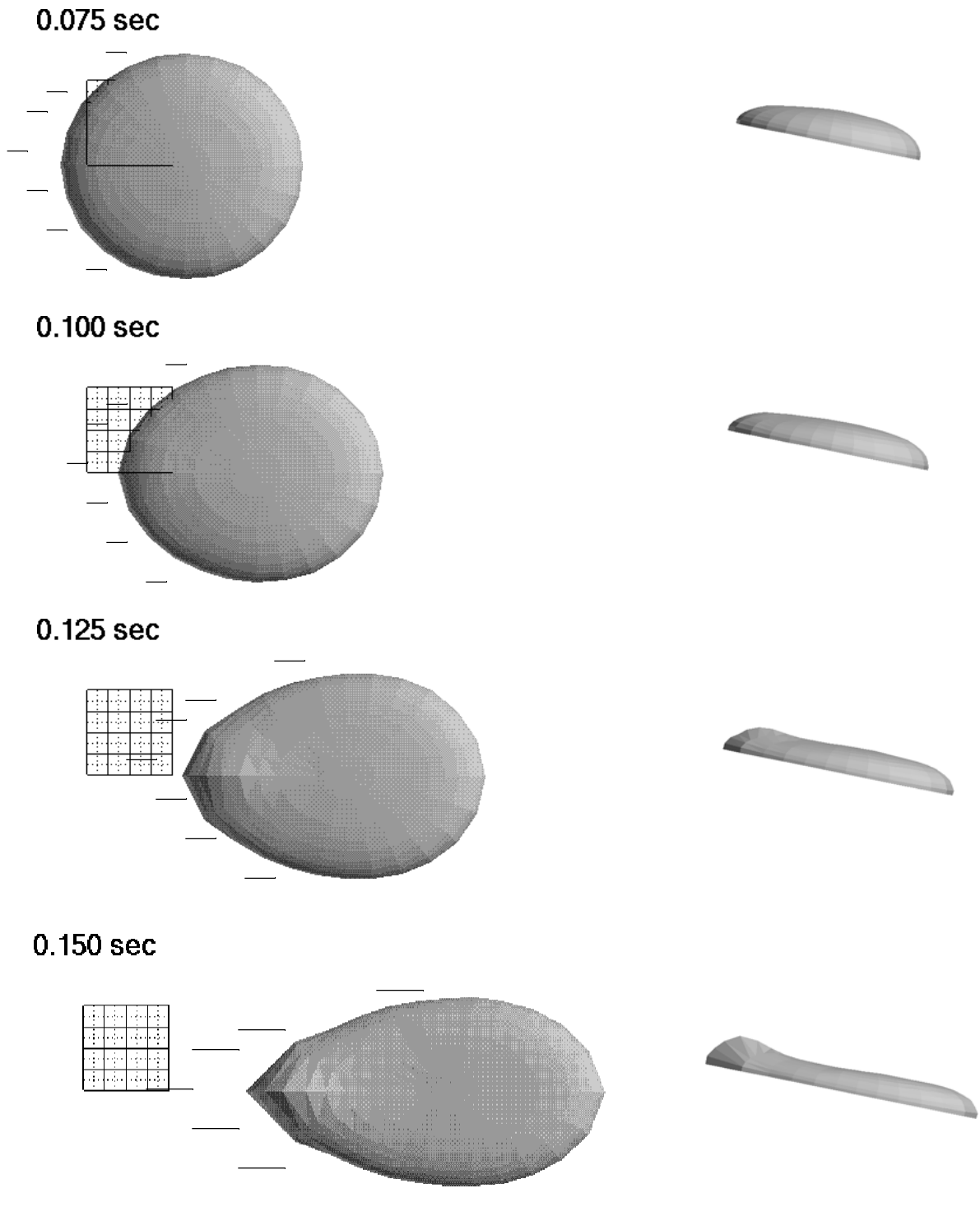


Figure 2. A sequence of time frames as the droplet starts to accelerate down the incline.

Distribution
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