Direct Numerical Simulations of Multiphase Flows-7

Results and Tests

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In this lecture we apply our code to a few problems and examine its performance. We will, specifically, look at

- A falling drop and its collision with a no-slip wall
- A rising bubble and its interaction with a no-slip wall
- The Rayleigh-Taylor instability in a domain with full slip vertical walls

We usually do our simulations in arbitrary computations units but report the results in non-dimensional units. For multi fluid flows we often encounter the following non dimensional numbers, where d and U stand for a length and a velocity scale. Symbols for the various physical quantities follow the usual convention.

Ohnsorge: $Oh = \frac{\mu}{\sqrt{\rho\sigma d}}$

Reynolds: $Re = \frac{\rho d U}{\mu}$

Archimedes: $N = \frac{\rho \Delta\rho g d^3}{\mu^2}$

Capillary: $Ca = \frac{\mu U}{\sigma}$

Weber: $We = \frac{\rho d U^2}{\sigma}$

Morton: $M = \frac{\Delta\rho g \mu^4}{\rho^2\sigma^3}$

Eötvös: (or Bond) $Eo = Bo = \frac{\Delta\rho g d^2}{\sigma}$

Froude: $Fr = \frac{\rho U^2}{\Delta\rho g d}$

A Falling Drop Hitting a Wall

For a falling drop, as well as a rising bubble, the velocity can be written as a function of the various parameters specifying the problem, as well as time

$$U = f(\rho_d, \mu_d, \Delta\rho g, \sigma, d, \rho_o, \mu_o, t)$$

Notice that we include gravity multiplied by the density difference, sine that is the effective buoyancy force. Using the diameter d, drop density, and density difference times gravity, as the repeated variables we find that the non-dimensional relationship is:

$$\frac{\rho U^2}{\Delta\rho g d} = f\left(\frac{\rho\Delta\rho g d^3}{\mu^2}, \frac{\Delta\rho g d^2}{\sigma}, \frac{\rho_d}{\rho_o}, \frac{\mu_d}{\mu_o}, \sqrt{\frac{t^2\Delta\rho g}{\rho d}}\right)$$

Or

$$Fr = f(N, Eo, r, m, \tau)$$

where

$$Fr = \frac{\rho U^2}{\Delta\rho g d}, \quad N = \frac{\rho\Delta\rho g d^3}{\mu^2}, \quad Eo = \frac{\Delta\rho g d^2}{\sigma}, \quad r = \frac{\rho_d}{\rho_o}, \quad m = \frac{\mu_d}{\mu_o}, \quad \tau = \sqrt{\frac{t^2\Delta\rho g}{\rho d}}$$

We can select other repeated variables to obtain other relationships, but in all cases the problem is specified by two non-dimensional numbers, plus the ratio of the densities and viscosities. The particular non-dimensional numbers selected usually depend on the various limiting cases we want to explore.

Sometimes we can ignore the dependency on the viscosity or surface tension, in which case the dynamics depends only on one non-dimensional number. If both can be ignored the problem is even simpler and is described by one non dimensional number being equal to a constant.

DNS of Multiphase Flows — Simple Front Tracking

This is the problem that we have been using to test our code, except here we will take the density and viscosity ratios to be larger. The physical and numerical parameters are specified in the first few lines of the code

```
%===============================================================
Lx=1.0; Ly=1.0; gx=0.0; gy=-100.0; sigma=10; % Domain size and
rho1=0.1; rho2=2.0; m1=0.01; m2=0.2;      % physical variables
unorth=0; usouth=0; veast=0; vwest=0; time=0.0;
rad=0.15; xc=0.5; yc=0.7;          % Initial drop size and location

%------------------- Numerical variables ---------------------
nx=32; ny=32; dt=0.001; nstep=200; maxit=200; maxError=0.001; beta=1.5; Nf=100;
```

This gives the following non-dimensional numbers:

Galileo Number

$$N = \frac{\rho \Delta \rho g d^3}{\mu^2} = \frac{2 \times 1.9 \times 1 \times 100 \times 0.3^3}{0.2^2} = 256.5$$

Eörtvös Number

$$Eo = \frac{\Delta \rho g d^2}{\sigma} = \frac{1.9 \times 100 \times 0.3^2}{10} = 1.71$$

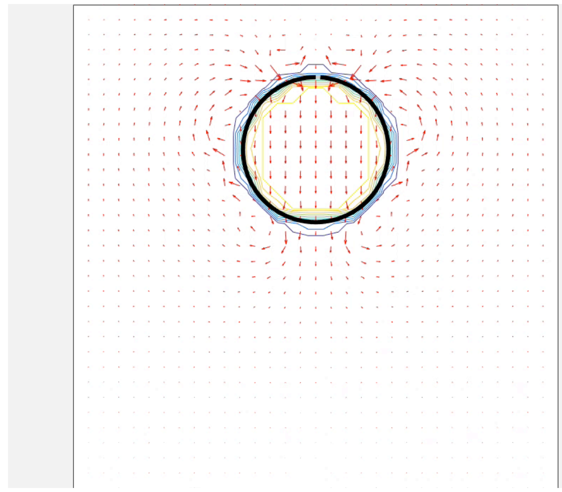
Property ratios

$$r = \frac{\rho_d}{\rho_o} = \frac{2.0}{0.1} = 20$$

$$m = \frac{\mu_d}{\mu_o} = \frac{0.2}{0.01} = 20$$

DNS of Multiphase Flows

Simulation of a drop that falls onto a rigid wall and bounces slightly



N=256.5
Eo=1.71
ρ_b/ρ_l=20
μ_b/μ_l=20

A 32 by 32 grid.

DNS of Multiphase Flows

For initial checks of the code, we can use relatively benign parameters, where we do not expect numerical difficulties and the resolution required for convergence is modest. Then we ask:

Does it look right?

Is the solution as symmetric as it should be?

Does rotating or flip the problem give the same solution?

Can we test some aspects of the code using analytical solutions?

Does the solution converge under grid refinement?

DNS of Multiphase Flows

Looking at how the velocity and the marker function evolve in time is usually the first step in examining the results. In many cases, however, we desire a more quantitative description of the evolution. This is useful for

- Assessing the convergence of the solution as the numerical parameters, such as the grid resolution, are varied
- Quantifying how the solution changes as the physical parameters describing the problem are changed

The diagnostic variables, or the quantities of interest, can be defined in several ways, but here we focus only on the simplest ones, such as the area of the drop and the location and velocity of its centroid

DNS of Multiphase Flows

The area of the drop should be constant since the flow is incompressible, and monitoring the area serves as a check on the accuracy of the computations.

To compute the area as well s several other quantities of interest it is often useful to convert the elementary definition as a volume or area integral to a surface integral since surface integrals can be found with a high degree of accuracy. Thus, the area is given by:

Area of drop

$$A = \int da = \int 1 da = \frac{1}{2}\int \Big(\frac{\partial x}{\partial x} + \frac{\partial y}{\partial y}\Big) da = \frac{1}{2}\int \nabla \cdot \mathbf{x} = \frac{1}{2}\oint \mathbf{x}\cdot\mathbf{n} ds$$

DNS of Multiphase Flows

Centroid of drop

$$\mathbf{X}_C = \frac{1}{A}\int \mathbf{x} da = \frac{1}{A}\int (x,y) da = \frac{1}{2A}\int \Big(\frac{\partial x^2}{\partial x}, \frac{\partial y^2}{\partial y}\Big) da$$
$$= \frac{1}{2A}\int \nabla \Big(x^2+y^2\Big) da = \frac{1}{2}\oint \Big(x^2+y^2\Big)\mathbf{n} ds$$

The velocity of the drop centroid can be found by differencing the location of the centroid

$$\mathbf{V}_C = \frac{d\mathbf{X}_C}{dt}$$

The velocity of the drop centroid can also be found by by integrating over the boundary, but this is usually less accurate.

Other elementary quantities of interest include the interface length which is found by

$$S = \oint ds$$

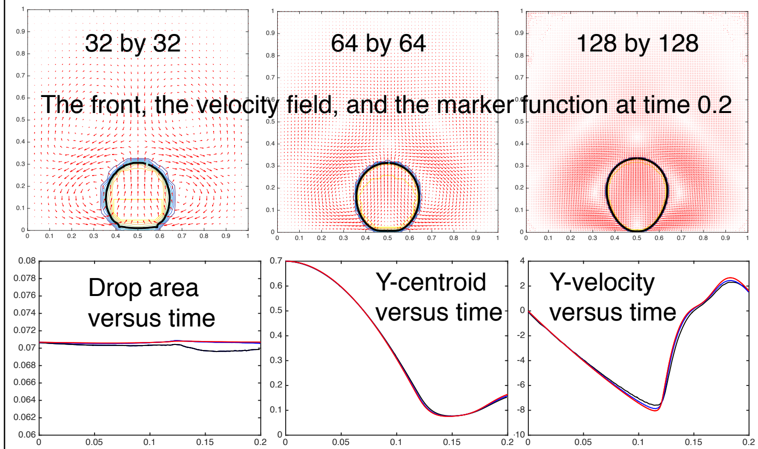
Here we use integration over the front to compute the area and the centroids. The code to do so is:

```
%================= DIAGNOSTICS =============================
  Area(is)=0; CentroidX(is)=0; CentroidY(is)=0; Time(is)=time;

  for j=1:Nf, Area(is)=Area(is)+...
      0.25*((xf(j+1)+xf(j))*(yf(j+1)-yf(j))-(yf(j+1)+yf(j))*(xf(j+1)-xf(j)));
    CentroidX(is)=CentroidX(is)+...
      0.125*((xf(j+1)+xf(j))^2+(yf(j+1)+yf(j))^2)*(yf(j+1)-yf(j));
    CentroidY(is)=CentroidY(is)-...
      0.125*((xf(j+1)+xf(j))^2+(yf(j+1)+yf(j))^2)*(xf(j+1)-xf(j));
  end
  CentroidX(is)=CentroidX(is)/Area(is);CentroidY(is)=CentroidY(is)/Area(is);

% plot(Time,Area,'r','linewidth',2); axis([0 dt*nstep 0 0.1]);
% set(gca,'Fontsize',18, 'LineWidth',2)
% T1=Time;A1=Area;CX1=CentroidX;CY1=CentroidY;
% T2=Time;A2=Area;CX2=CentroidX;CY2=CentroidY;
```


Results for three grids



A Rising Bubble Colliding with a Wall

A bubble is the inverse of a drop, where a light fluid blob moves in a heavy liquid. We will make the domain twice as long, so that the bubble will have time to reach an approximate steady state before hitting the top wall

```
Lx=1.0;Ly=2.0;gx=0.0;gy=-100.0; sigma=10; % Domain size and
rho1=2.0; rho2=0.05; m1=0.1; m2=0.005;    % physical variables
unorth=0;usouth=0;veast=0;vwest=0;time=0.0;
rad=0.15;xc=0.5;yc=0.3;       % Initial bubble size and location

%------------------- Numerical variables ---------------------
nx=32;ny=64;dt=0.00125;nstep=400; Nf=100;
maxit=200;maxError=0.001;beta=1.5;
```

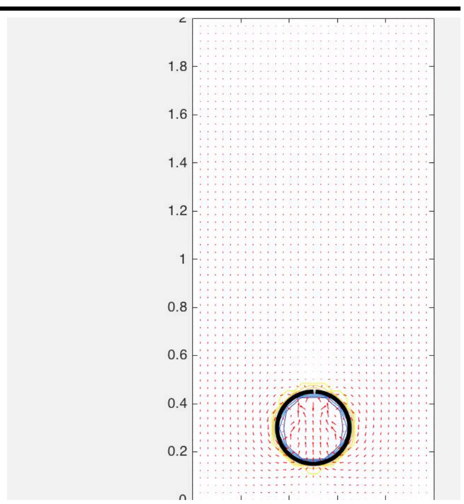
Galileo Number $$N = \frac{\rho \Delta \rho g d^3}{\mu^2} = \frac{2 \times 1.95 \times 100 \times 0.3^3}{0.1^2} = 1.053 \times 10^3$$

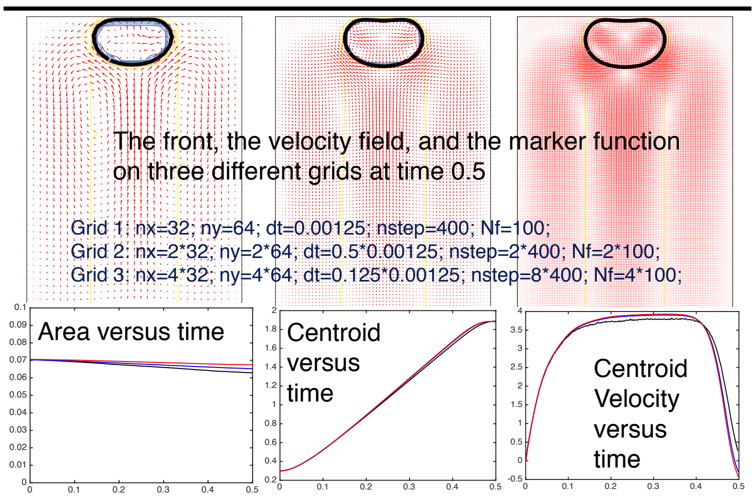
Eörtvös Number $$Eo = \frac{\Delta \rho g d^2}{\sigma} = \frac{1.95 \times 100 \times 0.3^2}{10} = 1.755$$

Simulation of a bubble rising in a narrow domain and colliding with the top rigid wall

$N=1.053 \times 10^3$
$Eo=1.755$
$\rho_b/\rho_l=40$
$\mu_b/\mu_l=20$

A 32 by 64 grid.





The Rayleigh-Taylor Instability

The Rayleigh-Taylor instability is one of the classical test problems for multiphase simulations. Initially a heavy fluid sits above a lighter one, but once the interface is perturbed slightly the heavy fluid and the light one trade places.

For this problem we need to change our code slightly:

- We change the boundary condition on the vertical walls to full-slip for the flow solver, and
- The front now stretches between the walls instead of being closed
- The boundary conditions for the front, where it meets the walls is simplified by assuming that the interface is flat there

Making the vertical walls full-slip is a very minor change. We want the shear stress there to be zero, so the velocity gradient is zero and this is accomplished by putting the tangent velocity at the ghost point equal to the first tangent velocity inside the domain.

The changes to the front are also relatively simple. The biggest decision is whether there is a front point on the boundary or whether we let put the boundary between the first point and the second one?

Here we choose to do the latter, so that the first and the last points are ghost points outside the computational domains.

The changes in the code are relatively minor. First of all, we modify the physical and numerical parameters slightly and change the initial conditions:

```
%============================================================
Lx=1.0;Ly=2.0;gx=0.0;gy=-100.0;  sigma=5.0; % Domain size and
rho1=1.0; rho2=4.0; m1=0.01; m2=0.05;          % physical variables
unorth=0;usouth=0;veast=0;vwest=0;time=0.0;

%-------------------- Numerical variables ---------------------
nx=32; ny=64; dt=0.00125; nstep=300;
maxit=200; maxError=0.001; beta=1.5; Nf=100;

%-------------------- Initial Conditions -----------------------
r=zeros(nx+2,ny+2)+rho1;m=zeros(nx+2,ny+2)+m1; % Set density and viscosity
for i=1:nx+2,for j=1:ny+2;                              % for the domain and the drop
  if(y(j)>1.2+0.1*cos(2.0*pi*x(i))), r(i,j)=rho2; m(i,j)=m2; chi(i,j)=1.0; end,
end, end
```


Then we need to change a few things

After finding the velocity, we add a line:
```
uf(2)=0; uf(Nf+1)=0; % Make sure the endpoint move along wall
```

After moving the points we change a line
```
xf(1)=-xf(2);yf(1)=yf(2);xf(Nf+2)=2*Lx-xf(Nf+1);yf(Nf+2)=yf(Nf+1);
```

After finding the marker function we add a line:
```
chi(1,:)=chi(2,:); chi(nx+2,:)=chi(nx+1,:); % Correct density on sides
```

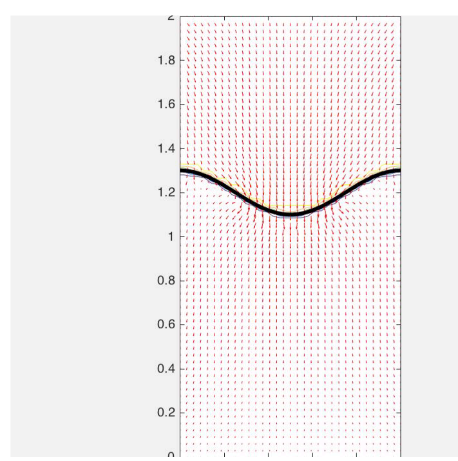
Before updating the velocities we modify the boundary conditions
```
v(1,1:ny+1)=v(2,1:ny+1);v(nx+2,1:ny+1)=v(nx+1,1:ny+1);
```

Before finding diagnostics we change a line
```
uf(1)=uf(2);vf(1)=vf(2);uf(Nf+2)=uf(Nf+1);vf(Nf+2)=vf(Nf+1); % Front
```

After adding and deleting points we change the updating of the ghost points
```
xf(1)=-xf(2);yf(1)=yf(2);xf(Nf+2)=2*Lx-xf(Nf+1);yf(Nf+2)=yf(Nf+1);
```

Change the plotting slightly:
```
plot(xf(1:Nf+2),yf(1:Nf+2),'k','linewidth',3);pause(0.01)
```


Simulation of a Rayleigh-Taylor instability where a heavy fluid falls into a lighter one.

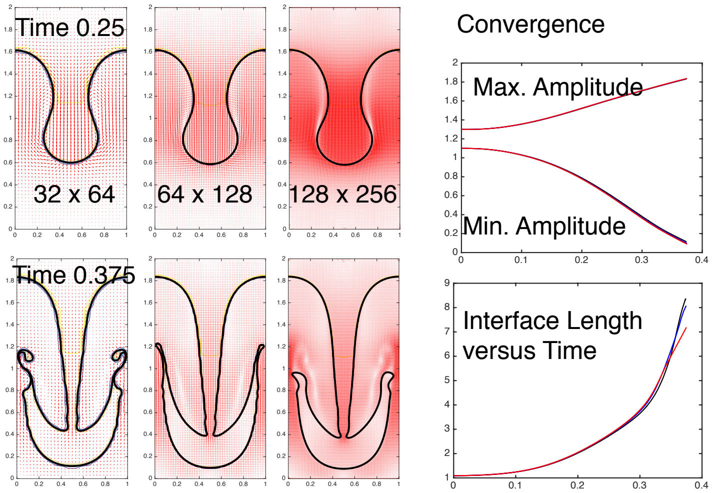


Nondimensional numbers based on the properties of the heavy fluid and d=1.

N=4.8 x 10^5
Eo=60
ρ_t/ρ_b=4
μ_t/μ_b=5

A 32 by 64 grid.

DNS of Multiphase Flows



DNS of Multiphase Flows

The current code can easily be modified for many other problems, such as waves, bubbles and drops coalescing with each other or an interface, and more than one bubble or drop.

The current code is written assuming a single continuous interface. For complex problems with many bubbles or drops, where there are several unconnected interfaces, a more general interface data structure is generally preferred.