Homework #7 (1 problem; 55 points)

due: April 10th, 2023.

Problem 7.1 [55]	Total

Problem 7.1 55 points:

Start with the code you have created for Problem 5.4. Keep the domain size ($L_x = 0.04\ m$ and $L_y = 0.02\ m$) boundary conditions unchanged.

a) Initialize one spherical droplet in the center of the domain and the corresponding level-set distance field (x coordinate of the droplet center is $x_d = 0.02\ m$). Droplet diameter is half domain height ($D_d = \frac{L_y}{2}$). Plot the initial droplet and the level set field with $N_y = 30$ and 50 elements across the domain height respectively. Use $M = 3$ in Eq. (3.53) and (3.54). [5 points]

b) Implement variable property in your solver (ρ and μ are now arrays instead of just constants, and you will also need to modify your predictor & corrector steps accordingly to incorporate variable density and viscosity). Set liquid density, viscosity as $\rho_l = 10^3 \frac{kg}{m^3}, \mu_l = 10^{-3}\ Pa\ s$, and gas density, viscosity as $\rho_g = 1 \frac{kg}{m^3}, \mu_g = 10^{-5}\ Pa\ s$. Plot your initial density and viscosity distribution with $N_y = 30$ and 50. [10 points]

c) Initialize the velocity field to be the **analytical solution** and **advect** the droplet through $\sim 20\%$ of the domain length, i.e., $0.008\ m$. The advection procedure is described in Eqns. (3.41) – (3.46). Plot the advected droplet and the distance field with $N_y = 30$ and 50 elements across the domain height respectively. Compare and discuss the advected droplet shape with the initial one. [10 points]

Note:

- Reduce your time step size if needed.
- Do not implement the re-initialization, you will implement it in d)
- Do not implement surface tension, you will implement it in e)

d) Add the re-initialization steps into the solver. **Advect** the droplet through $\sim 20\%$ of the domain length with $N_y = 50$ elements across the domain. **Compare and discuss** the distance fields with and without re-initialization. [10 points]

Note: refer to Eq. (3.48)-Eq. (3.53), Problem 6.1, Problem 6.2, and p. 60-61 of the textbook.

e) Implement the surface tension force in your solver. Use surface tension coefficient $\gamma = 0.06\ N/m$. **Advect** the droplet through $\sim 20\%$ of the domain length. Start with using $N_y = 30$ elements across the domain height and then increase the number of elements until $N_y = 120$ at your own pace. Plot the distance and pressure fields with at least two different element numbers besides 30 and 120 and **discuss** your result. [10 points]

Note: refer to Eq. (3.55), Eq. (3.56), as well as Eq. (3.8), Eq. (3.11), and Pages 61-62 of the textbook.

Extra Credit Use variable properties in Table 1 for liquid and gas and update the solver (you will obtain a two-phase solver using the "one-fluid" approach). **Advect** the droplet through $\sim 20\%$ of the domain length and pick two N_y element numbers you tested in e). Plot distance fields with at least 4 different combinations of two-phase properties and discuss how the contrast of properties affect your results. [10 points]

Table 1 Two-phase properties

	Density (ρ) kg/m^3	Dynamic viscosity (μ) $Pa\ s$
Liquid (droplet)	10^3	1×10^{-3}
Gas	9.99×10^2, 10^2, 10, 1	9×10^{-4}, 1×10^{-4}, 1×10^{-5}

Notes:

1) Refer to Eq. (3.12)-Eq. (3.13) and Pages 61-62 of the textbook.

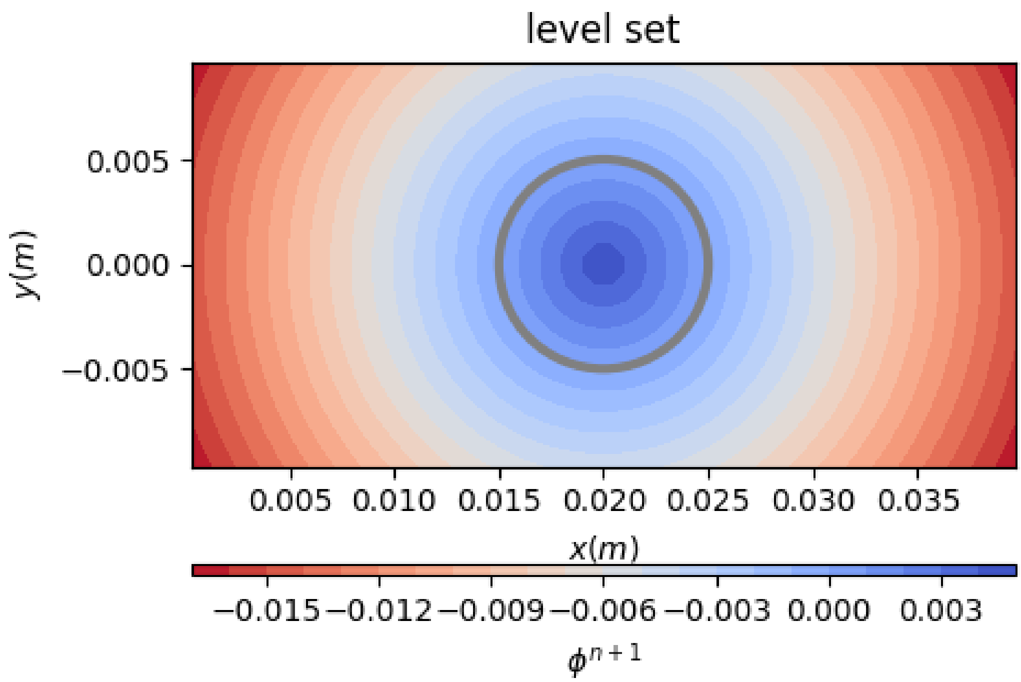
2) If you need to further increase the properties in Table 1, you can increase viscosity first, and then density.

General notes:

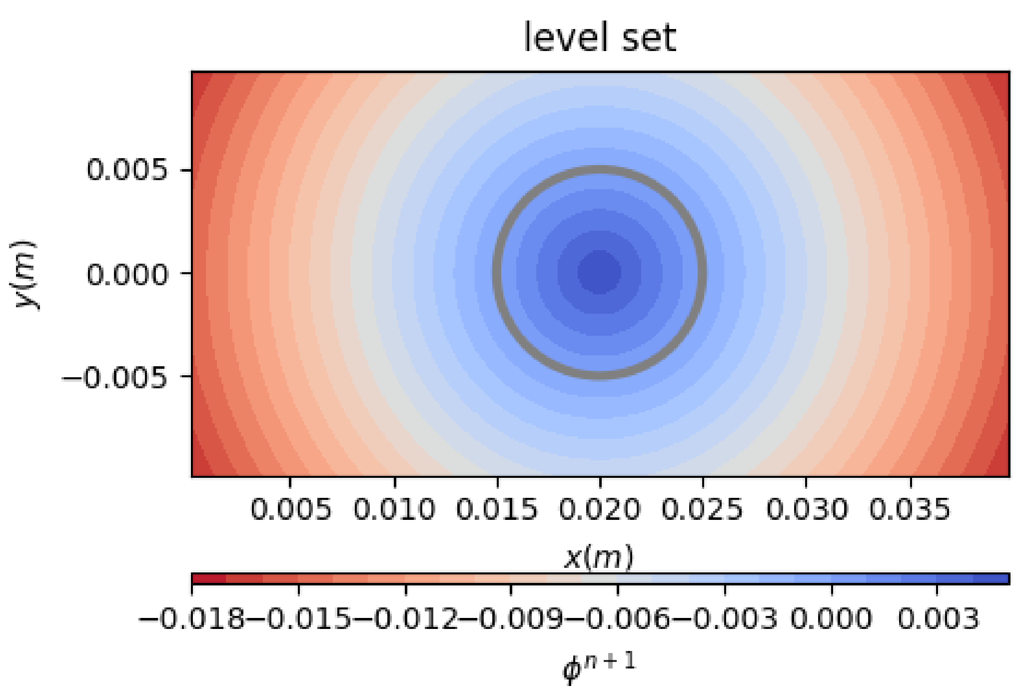
1) To expedite your coding and save trouble for debugging, write functions for all the operators (**strongly recommended!**).
2) Submit your code.

a) The initial level set field $\phi^n(\vec{x}, t = 0)$. The initial location of the interface is indicated as the gray circle.

$N_y = 30$:

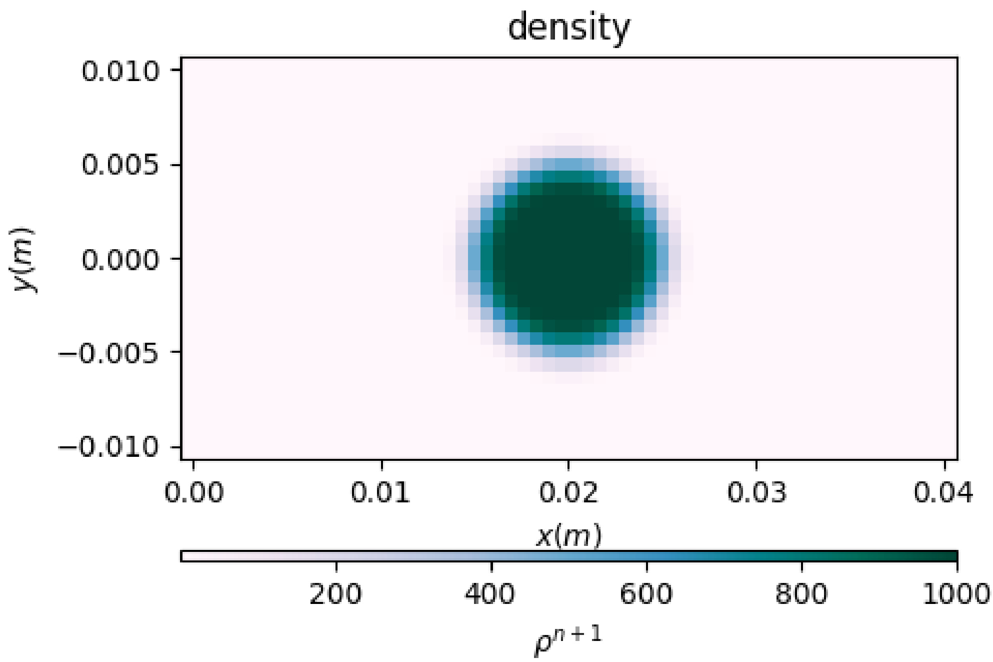


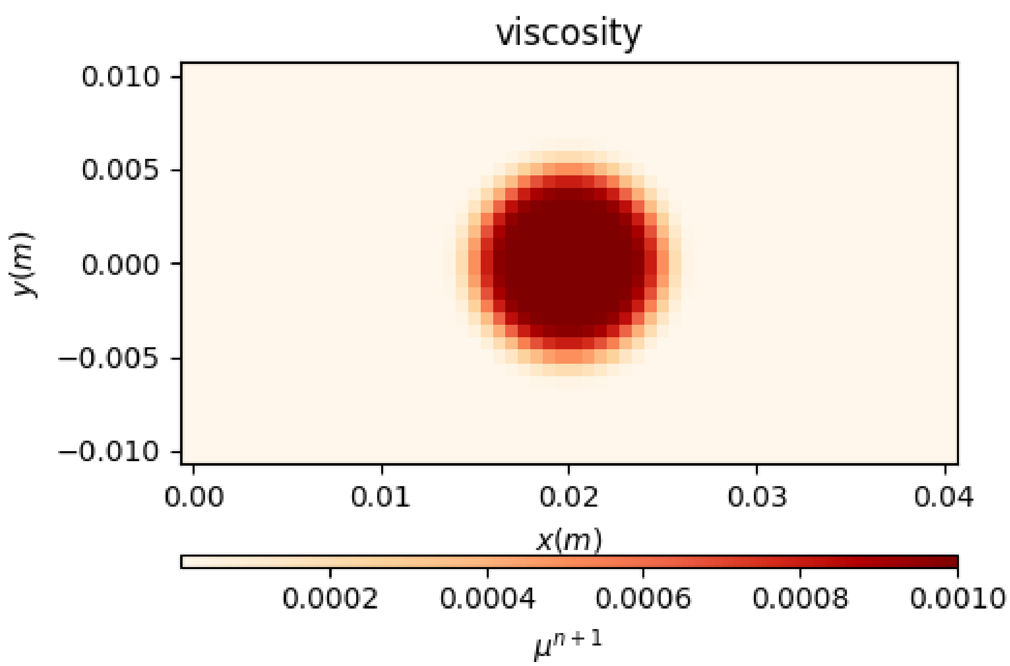
$N_y = 50$:



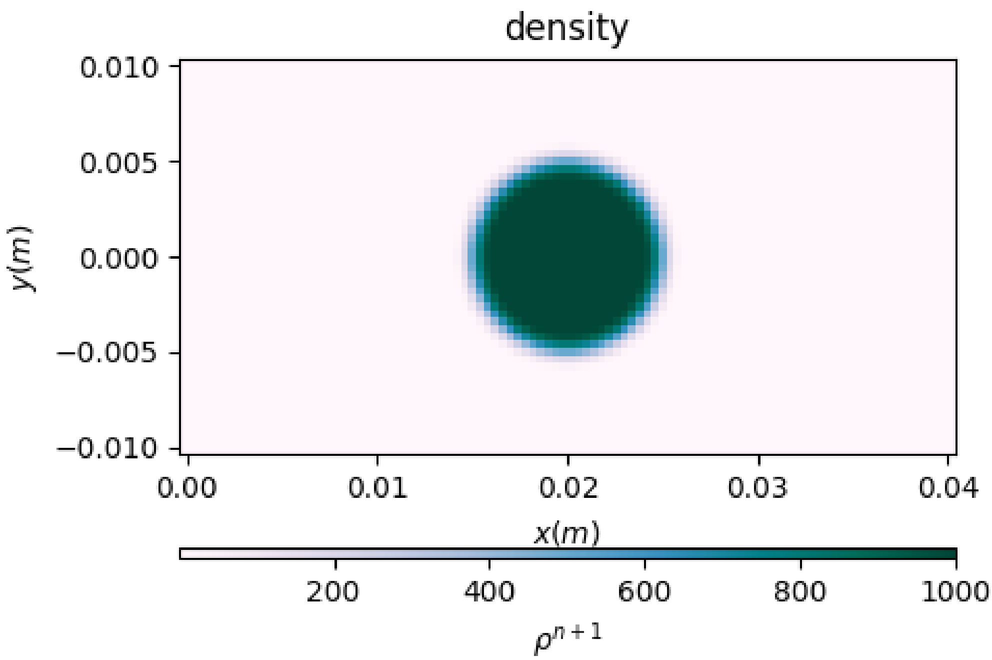
b) The density and viscosity distribution:

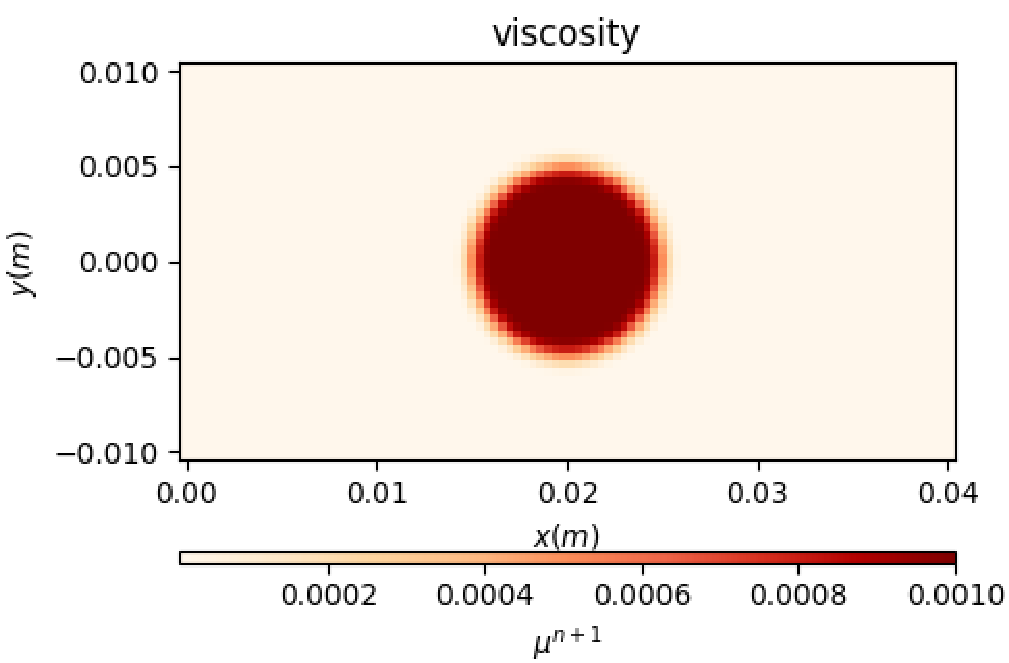
$N_y = 30$:





$N_y = 50$:





To incorporate variable density and viscosity, you will need to do the following after level set initialization:

1. Calculate $f(\phi)$ and calculate distribution of density and viscosity by:

$$\rho(\phi) = \rho_l f(\phi) + \rho_g(1 - f(\phi))$$

$$\mu(\phi) = \mu_l f(\phi) + \mu_g(1 - f(\phi))$$

2. Update your flow driving force term, advection step, pressure iteration and corrector step to use local ρ and μ:

   For predictor and corrector steps, the properties are the function of ϕ at the velocity locations (edges of pressure cells)

$$\frac{dp}{dx}\left(\phi_{i+\frac{1}{2},j}\right) = -2\mu\left(\phi_{i+\frac{1}{2},j}\right) u_{1,max}\left(\frac{2}{L_y}\right)^2$$

$$u^*_{i+\frac{1}{2},j} = u^n_{i+\frac{1}{2},j} + \Delta t\left[-A^n_{i+\frac{1}{2},j} + \frac{\mu\left(\phi_{i+\frac{1}{2},j}\right)}{\rho\left(\phi_{i+\frac{1}{2},j}\right)} D^n_{i+\frac{1}{2},j} - \frac{1}{\rho\left(\phi_{i+\frac{1}{2},j}\right)} \frac{dp}{dx}\left(\phi_{i+\frac{1}{2},j}\right)\right]$$

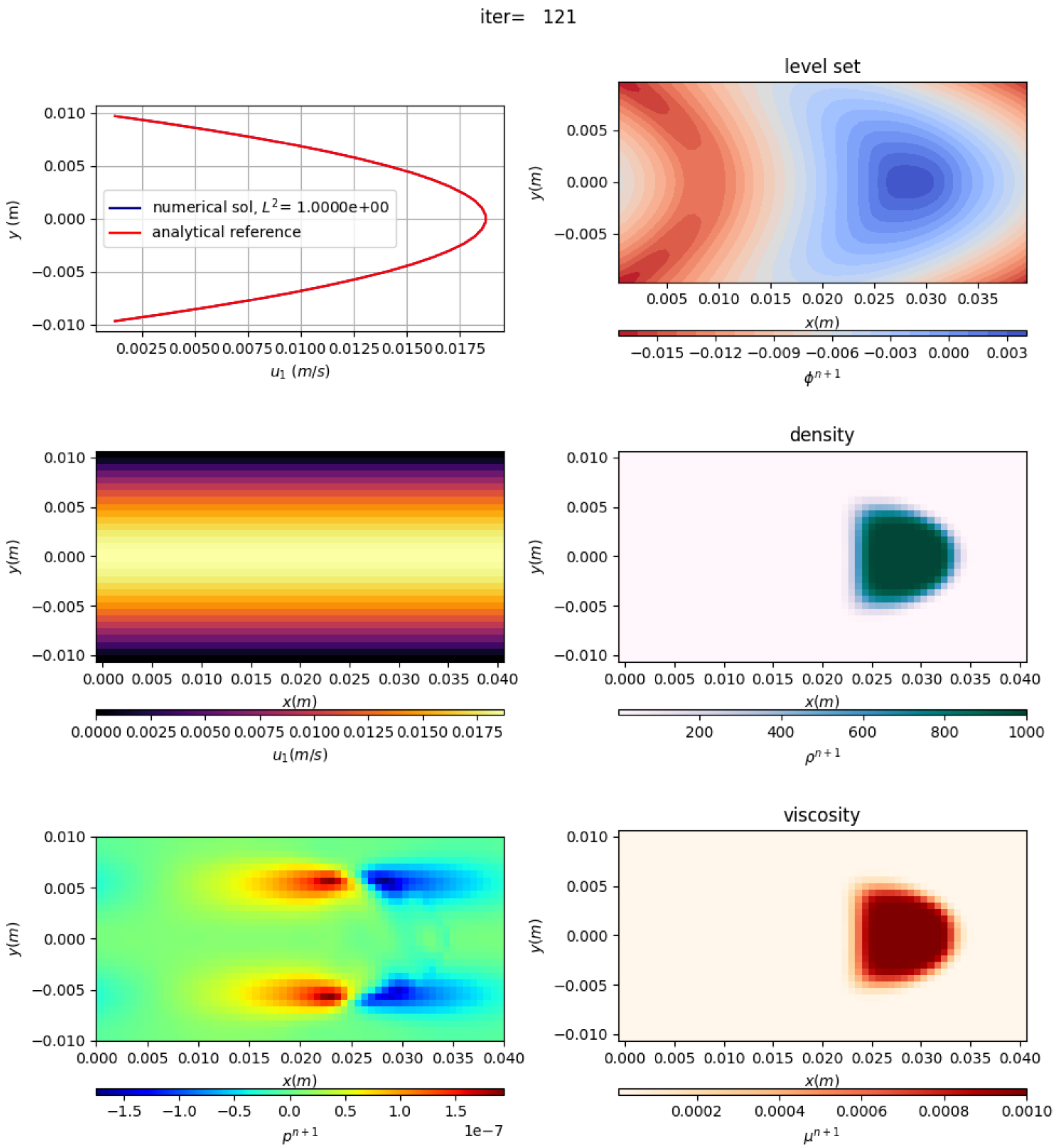
$$u^{n+1}_{i+\frac{1}{2},j} = u^*_{i+\frac{1}{2},j} - \frac{\Delta t}{\rho\left(\phi_{i+\frac{1}{2},j}\right)} \frac{p_{i+1,j} - p_{i,j}}{h}$$

   For pressure iteration, the density is the function of ϕ values at the cell center.

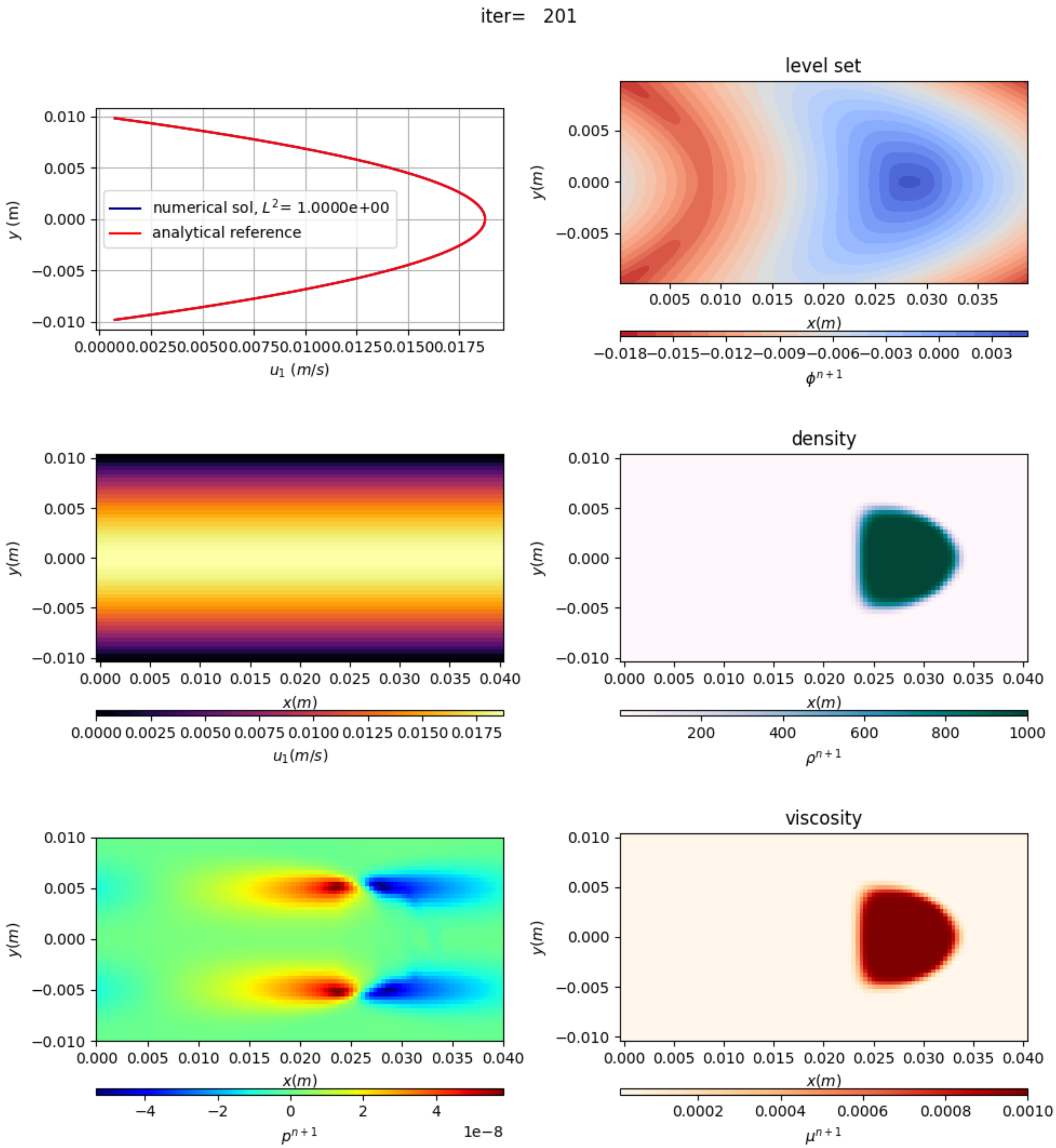
$$p^{n+1}_{i,j} = \left[\frac{h\rho(\phi_{i,j})}{\Delta t}\left(u^*_{i+\frac{1}{2},j} - u^*_{i-\frac{1}{2},j}\right) - (p^n_{i+1,j} + p^n_{i-1,j} + p^n_{i,j+1} + p^n_{i,j-1})\right] / (-4)$$

c) Distribution of solution variables and properties with level set advection:

$N_y = 30$:



$N_y = 50$:



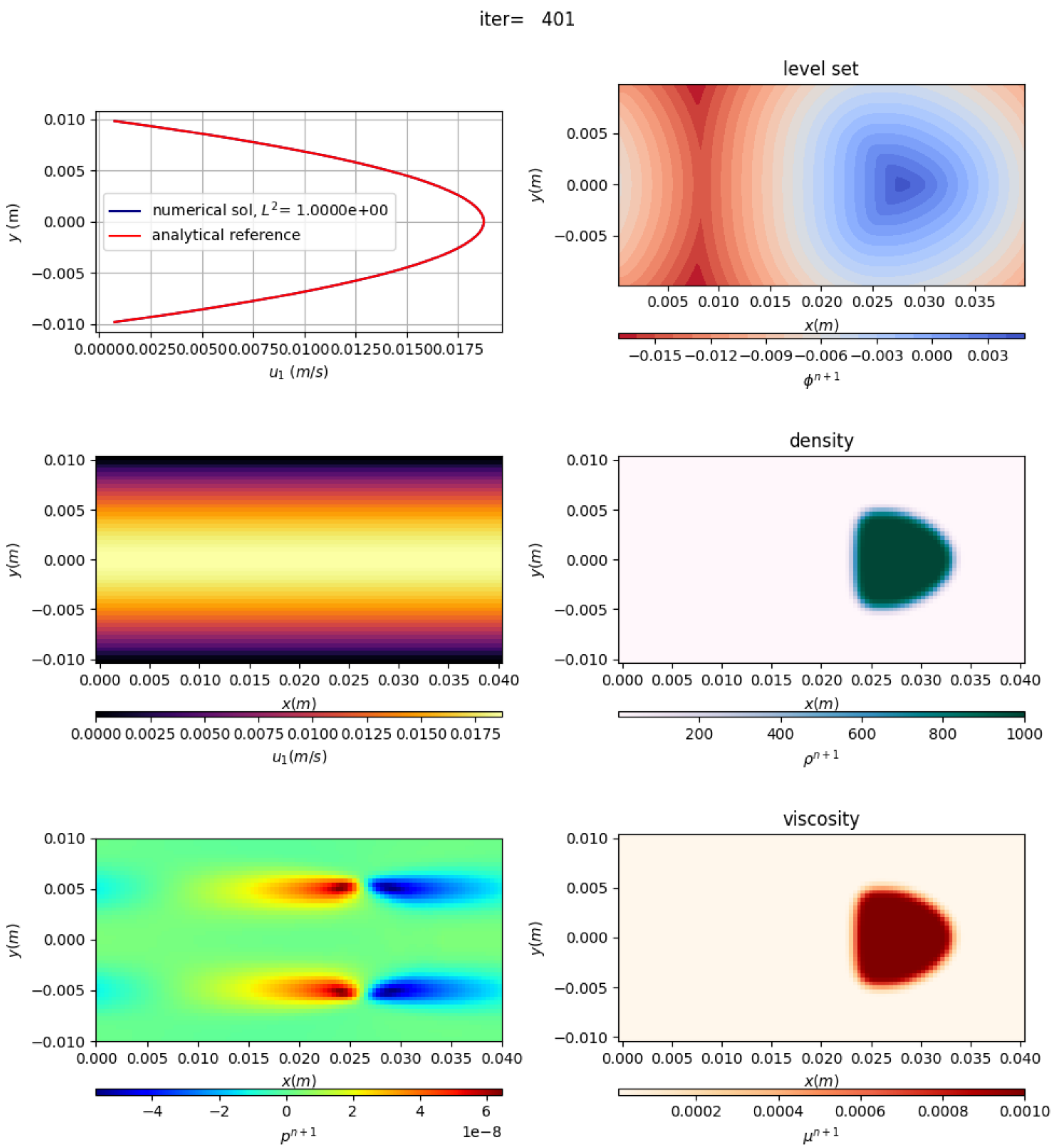
iter= 201
numerical sol, L^2= 1.0000e+00
analytical reference
y (m)
u_1 (m/s)
level set
y(m)
x(m)
ϕ^{n+1}
density
ρ^{n+1}
$u_1(m/s)$
viscosity
μ^{n+1}
p^{n+1}
1e−8

Discussion:

The droplet is being advected by the local velocity by $\sim 0.008\ m$ after a few steps. Compared to the initial state, the droplet deformed into bell shape due to the local shear, as can be clearly seen from the level set and property distribution. Due to the same reason, the level set field is severely distorted near the walls and the gradient of ϕ is clearly deviated from 1.0, which does not satisfy the requirements as a distance field. Inside the droplet, the level set field is slightly elongated.

As we increase the number of elements across the walls from $N_y = 30$ to $N_y = 50$, the property transition region becomes sharper as the element spacing reduces and the droplet is better resolved.

d) Distribution of solution variables and properties with level set advection and re-initialization step:

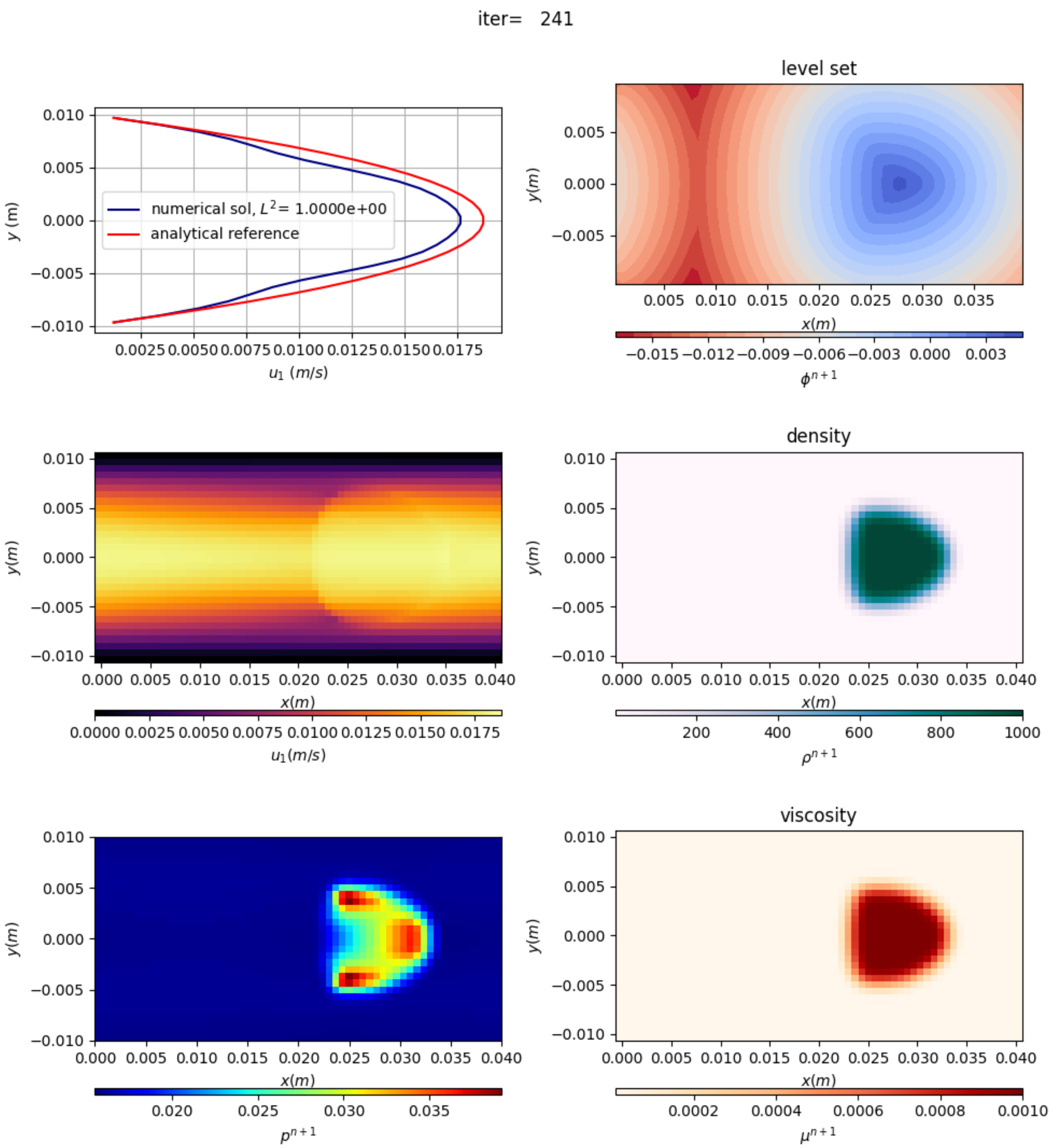


Discussion:

With the re-initialization operation, the correctness of the distance field distribution is reinstated. As one can see, the gradient of the level set field normal to the interface is now close to one inside and outside the droplet and the strong distortion near the wall and the elongation within the droplet has been corrected. The shape of the droplet, however, does not change after the re-initialization.

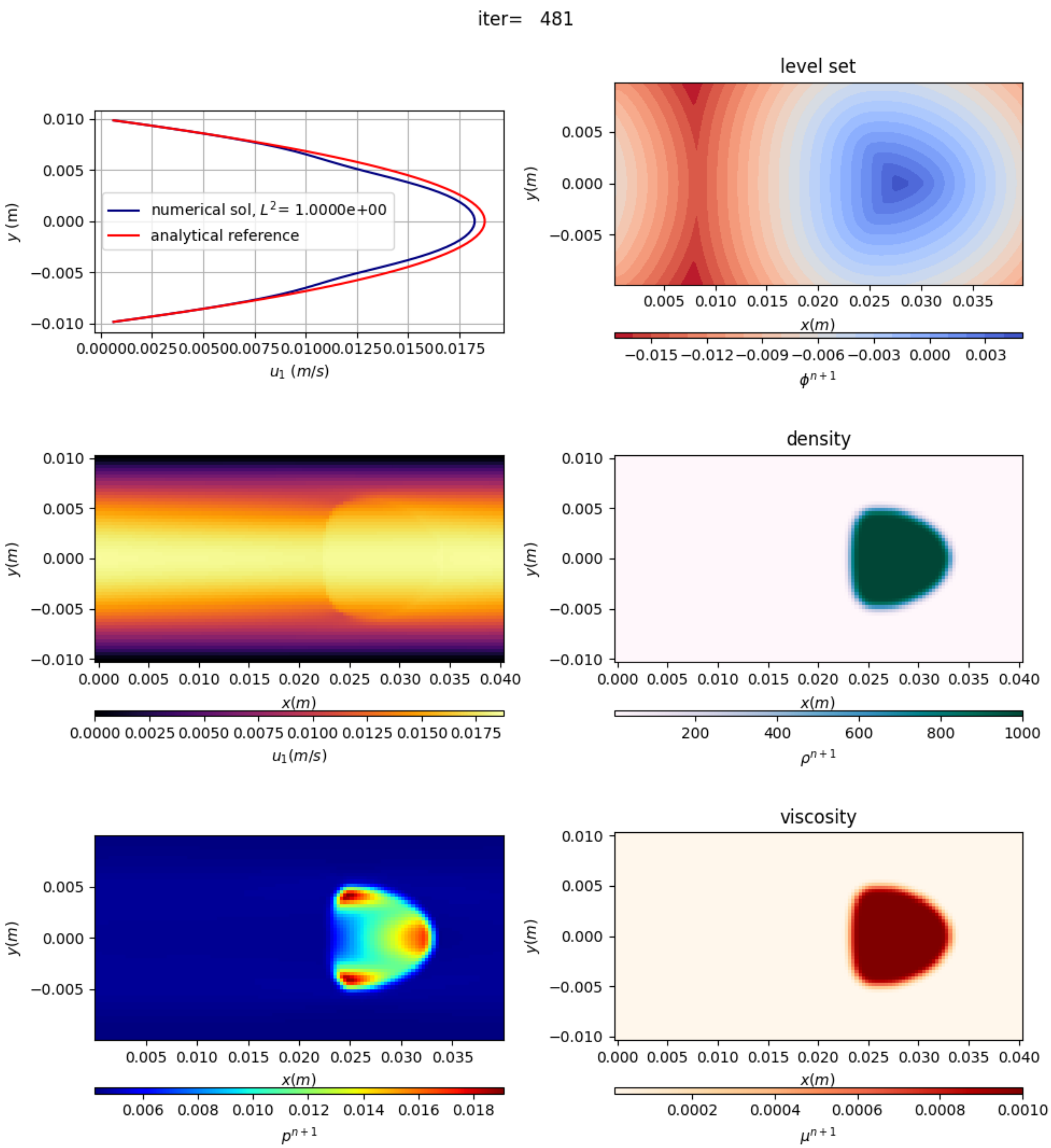
e) Distribution of solution variables and properties with level set advection, re-initialization step and surface tension:

$N_y = 30$:

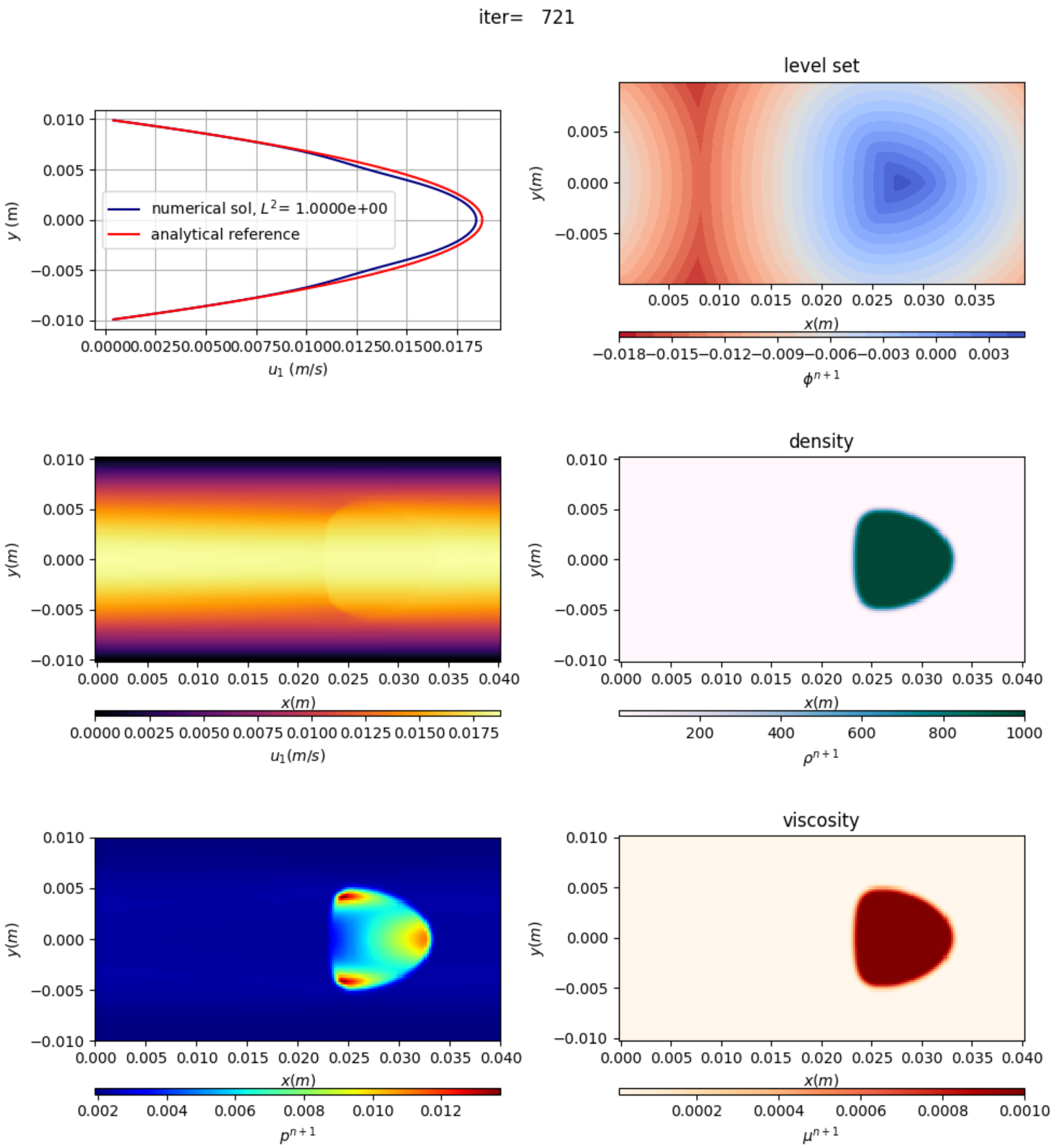


iter= 241
numerical sol, L^2= 1.0000e+00
analytical reference
y (m)
u_1 (m/s)
level set
$y(m)$
$x(m)$
ϕ^{n+1}
$u_1(m/s)$
density
ρ^{n+1}
p^{n+1}
viscosity
μ^{n+1}

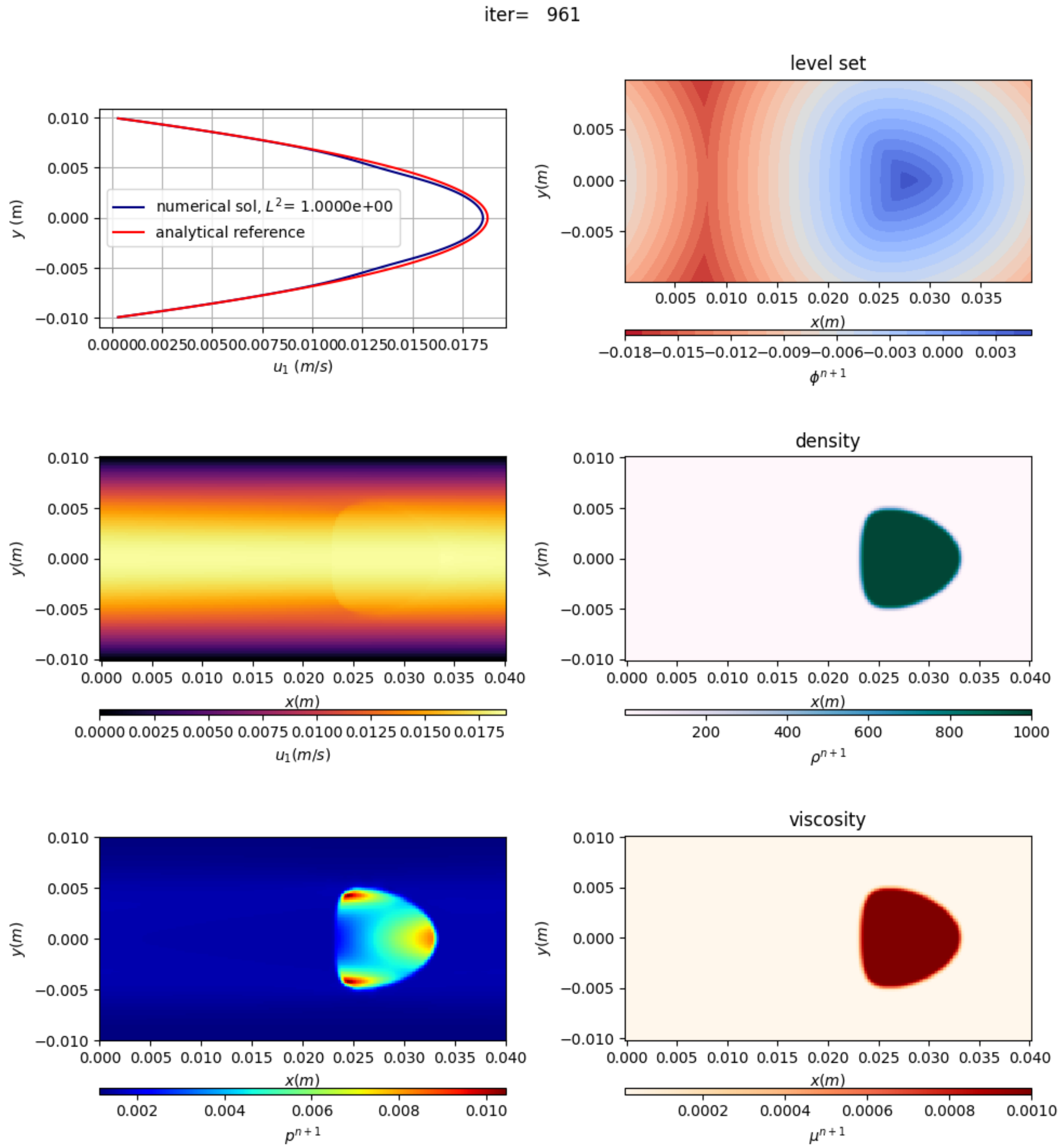
$N_y = 60$:


iter= 481
numerical sol, L^2= 1.0000e+00
analytical reference
y (m)
u_1 (m/s)
level set
x(m)
y(m)
ϕ^{n+1}
$u_1(m/s)$
density
ρ^{n+1}
p^{n+1}
viscosity
μ^{n+1}

$N_y = 90$:


iter= 721
numerical sol, L^2= 1.0000e+00
analytical reference
y (m)
u_1 (m/s)
level set
y(m)
x(m)
ϕ^{n+1}
density
ρ^{n+1}
$u_1(m/s)$
viscosity
μ^{n+1}
p^{n+1}

$N_y = 120$:



Discussion:

With the surface tension, one will first see the pressure increase inside the droplet in the beginning of the simulation. After the droplet is advected for $\sim 0.008\ m$ the pressure inside the droplet redistributed and has higher value towards the tip and the two lateral ends. Compared to the shape without surface tension, the droplet is squeezed along the x direction slightly and the interface becomes rounder on the two lateral ends. As we refines the resolution, the pressure distribution inside the droplet is better resolved and the droplet property distribution is better represented.

Pseudo code for the solver: (color code for the actions required by **a)**, **b)**, **c)**, **d)**, **e)**

1. Simulation parameters specification (geometry (L_x, L_y), number of pressure cells (N_x, N_y), fluid properties ($\rho_l, \rho_g, \mu_l, \mu_g, \gamma$), given flow conditions($u_{max}, \frac{dp}{dx}$), max number of iterations ($n_{iter,max}$), Δt (can be determined by CFL since u_{max} is known), pressure iteration tolerance $\epsilon_{p,tol}$, max number of pressure iteration ($n_{piter,max}$), level set-related parameters ($M, \tau, \Delta\tau$), droplet geometry (D_d, x_d, y_d)
2. Functions for surface tension, level set advection and re-distancing operations:

$$M(a,b), f(\phi), D_x^+, D_x^-, D_x^+ D_x^-, L\phi^n, L\phi^*, sgn(\phi), sgn_{Mh}(\phi), \widetilde{D}_x^+, \widetilde{D}_x^-, \widetilde{D}_y^+, \widetilde{D}_y^-, L\phi_d^n, L\phi_d^*$$

$$\kappa(\phi), \frac{df(\phi)}{d\phi}, \nabla\phi$$

3. Data array declaration and initialization (e.g., cell center coordinates, x-velocity, pressure p, level set ϕ, re-distancing field ϕ_d, density ρ, viscosity μ, reference x-velocity
4. Initialization:

$$u = u_{ini}$$

$$\phi = r_d - \sqrt{(x - x_d)^2 + (y - y_d)^2}$$

$$\rho(\phi), \mu(\phi)$$

5. While ($n_{iter} < n_{iter,max}$): (in this homework n_{iter} is determined by length of advection)

   - Enforce B.C. for u^n

   - Predictor step for all cells:

$$\frac{dp}{dx}\left(\phi_{i+\frac{1}{2},j}\right) = -2\mu\left(\phi_{i+\frac{1}{2},j}\right) u_{1,max}\left(\frac{2}{L_y}\right)^2$$

$$f_{st,x}\left(\phi_{i+\frac{1}{2},j}\right) = \gamma\kappa\left(\phi_{i+\frac{1}{2},j}\right)\frac{df}{d\phi}\nabla_x\phi_{i+\frac{1}{2},j}$$

$$u^*_{i+\frac{1}{2},j} = u^n_{i+\frac{1}{2},j} + \Delta t\left[-A^n_{i+\frac{1}{2},j} + \frac{\mu\left(\phi_{i+\frac{1}{2},j}\right)}{\rho\left(\phi_{i+\frac{1}{2},j}\right)} D^n_{i+\frac{1}{2},j} - \frac{1}{\rho\left(\phi_{i+\frac{1}{2},j}\right)}\frac{dp}{dx}\left(\phi_{i+\frac{1}{2},j}\right)\right.$$

$$\left. - \frac{1}{\rho\left(\phi_{i+\frac{1}{2},j}\right)} f_{st,x}(\phi_{i+\frac{1}{2},j})\right]$$

- Enforce B.C. for u^*
- pressure iteration loop (solve for pressure):

While ($maxval(\epsilon_p) > \epsilon_{p,tol}$ && $n_{piter} < n_{piter,max}$):

for ($i = 1, i < Nx + 2, i++$): (each column of the domain)

$$RHS = \frac{\rho(\phi_{i,j})}{\Delta t}\left(\frac{u^*_{i+\frac{1}{2},j} - u^*_{i-\frac{1}{2},j} + v^*_{i,j+\frac{1}{2}} - v^*_{i,j-\frac{1}{2}}}{h}\right)$$

$$P^{n+1}_{i,j} = \frac{-1}{3}[h^2 * RHS - \left(p^n_{i+1,1} + p^n_{i-1,1} + p^n_{i,2}\right)]$$

$$RHS = \frac{\rho(\phi_{i,j})}{\Delta t}\left(\frac{u^*_{i+\frac{1}{2},j} - u^*_{i-\frac{1}{2},j} + v^*_{i,j+\frac{1}{2}} - v^*_{i,j-\frac{1}{2}}}{h}\right)$$

$$P^{n+1}_{i,j} = \frac{-1}{3}[h^2 * RHS - \left(p^n_{i+1,N_y} + p^n_{i-1,N_y} + p^n_{i,N_y-1}\right)]$$

for ($j = 2, j < Nx, j++$): (rows that are not adjacent to the walls)

$$RHS = \frac{\rho(\phi_{i,j})}{\Delta t}\left(\frac{u^*_{i+\frac{1}{2},j} - u^*_{i-\frac{1}{2},j} + v^*_{i,j+\frac{1}{2}} - v^*_{i,j-\frac{1}{2}}}{h}\right)$$

$$P^{n+1}_{i,j} = \frac{-1}{4}[h^2 * RHS - \left(p^n_{i+1,j} + p^n_{i-1,j} + p^n_{i,j-1} + p^n_{i,j+1}\right)]$$

Compute ϵ_p for each pressure cell $\epsilon_p = p^{n+1} - p^n$

Evaluate the maximum ϵ_p overall:

$$\epsilon_{p,max} = maxval(\epsilon_p)$$

Assign new pressure values to the old one:

$$p^n = p^{n+1}$$

Enforce pressure periodicity for p^{n+1}:

$$p_{0,j}^{n+1} = p_{Nx,j}^{n+1}$$

$$p_{N_x+1,j}^{n+1} = p_{1,j}^{n+1}$$

$$j \in [1, N_y]$$

Plus one to the pressure iteration count:

$$n_{piter} += 1$$

-Corrector step for all cells:

$$u_{i+\frac{1}{2},j}^{n+1} = u_{i+\frac{1}{2},j}^{*} - \frac{\Delta t}{\rho\left(\phi_{i+\frac{1}{2},j}\right)} \frac{p_{i+1,j} - p_{i,j}}{h}$$

-Level set advection:

Predictor step:

$$\phi_{i,j}^{*} = \phi_{i,j}^{n} + \Delta t \, (L\phi_{i,j}^{n})$$

Enforce periodicity for $\phi_{i,j}^{*}$

Corrector step:

$$\phi_{i,j}^{n+1} = \phi_{i,j}^{n} + \frac{\Delta t}{2} \, (L\phi_{i,j}^{n} + L\phi_{i,j}^{*})$$

Enforce periodicity for $\phi_{i,j}^{n+1}$

-Level set re-initialization:

$\phi_d^n = \phi^{n+1}$

while ($\tau \leq Mh$):

Predictor step:

$$\phi_d^* = \phi_d^n + \Delta\tau L\phi_d$$

Enforce periodicity for ϕ_d^*

Corrector step:

$$\phi_d^* = \phi_d^n + \frac{\Delta\tau}{2}(L\phi_d^n + L\phi_d^*)$$

Enforce periodicity for ϕ_d^{n+1}

$\phi^n = \phi_d^{n+1}$

-Update property distribution based on the new level set field

-Update n_{iter}, simulation time, convergence metrics, etc.

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