GESAR
The Group for Environmental Studies in Reservoirs

FEMSIM - FINITE ELEMENT METHOD SIMULATOR

3rd Workshop on Advances in CFD and LB Modelling of Interface Dynamics in Capillary Two-Phase Flows

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http://www.uerj.br http://2phaseflow.org

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Kobe - Japan
October 10th, 2018

OUTLINE

- Bibliography;
- Intro to femSIM2d;
- interface modeling;
- mesh storage;
- remeshing;
- code structure in C++
- the Python API
- Tasks: 2D examples;

BIBLIOGRAPHY

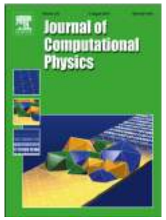
PhD thesis

A 3D ALE Finite Element Method for Two-Phase Flows with Phase Change
Thèse no. 5426 2012
EPFL, 2012

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

JCP article

3D Moving Mesh Finite Element Method for Two-Phase Flows
Journal of Computational Physics
2014



BIBLIOGRAPHY

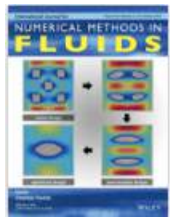
PhD thesis

Numerical Modelling of Two-Phase Flow with Moving Boundary Fitted Meshes
Thèse no. 8538 2018
EPFL, 2018

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

IJNMF article

Interface-Fitted Moving Mesh Method for Axisymmetric Two-Phase Flow in Microchannel
International Journal for Numerical Method in Fluids, 2017



OPEN SOURCE APPS

Below is a list of recommended softwares for visualization, text editing, mesh generation, linear system solvers and APIs. All softwares are **open source**.

- Paraview - 2D and 3D rendering
- Vim - text editor
- Boost-Python - C++/Python bindings
- PETSc - data structure and linear solvers
- tetgen - tetrahedral mesh generator
- triangle - triangular mesh generator
- Gmsh - 2D and 3D mesh generator
- gnuplot - portable command line graphic utility
- git - git repository (see github)

UNIX COMMANDS

```
/
├── /root
├── /usr
│   ├── /usr/include
│   └── /usr/lib
├── /opt
├── /home
│   └── /home/workshop
└── /bin
```

- pwd - check the current path
- ssh - connect to another machine
  - Ex.: ssh username@IPaddress
- cd - change directory:
  - Ex.: cd $HOME/projects
- ls - list files and folders
  - Ex.: ls -l
  - ls -G (for coloring - mac users)
- mv - move files:
  - Ex.: mv oldfilename newfilename
- vim - text editor:
  - Ex.: vim filename
- tail - show the last few lines of file:
  - Ex.: tail filename
- head - show the first few lines of file:
  - Ex.: head filename
- find - find files by name:
  - Ex.: find . -name aaa.txt
- alias - rename command
  - Ex.: alias ls = 'ls -G'
- in gnuplot:
  - Ex.: plot 'filename.dat' using 1:2

KOBE COMPUTERS

```
/
└── /home
    └── /home/workshop
        └── /home/workshop/projects/python/femSIM2d
            └── /home/workshop/projects/python/femSIM2d/<<case>>
                ├── vtk
                ├── dat
                └── msg
```


GOVERNING EQUATIONS

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{c} \cdot \nabla \mathbf{v} = -\frac{1}{\rho(\phi)} \nabla p + \frac{1}{Re} \nabla \cdot \left[\mu(\phi)(\nabla \mathbf{v} + \nabla \mathbf{v}^T)\right] + \frac{1}{Fr^2}\mathbf{g} + \underbrace{\frac{1}{We}\mathbf{f}}_{\text{surface tension}}$$

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial T}{\partial t} + \mathbf{c} \cdot \nabla T = \frac{1}{RePr} \nabla \cdot (k(\phi) \nabla T)$$

ALE formulation: $\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} - \hat{\mathbf{v}}) \cdot \nabla \mathbf{v} \begin{cases} \hat{\mathbf{v}} = \mathbf{v} \longrightarrow \text{Lagrangian} \\ \hat{\mathbf{v}} = 0 \longrightarrow \text{Eulerian} \end{cases}$

GOV EQ - AXISYMMETRIC

$$\frac{\partial v_x}{\partial t} + \mathbf{c}\cdot\nabla v_x = -\frac{1}{\rho(\phi)}\frac{\partial p}{\partial x} + \frac{1}{Re}\mu(\phi)\nabla^2 v_x + \frac{1}{Fr^2}g_x + \frac{1}{We}f_x$$

$$\frac{\partial v_r}{\partial t} + \mathbf{c}\cdot\nabla v_x = -\frac{1}{\rho(\phi)}\frac{\partial p}{\partial x} + \frac{1}{Re}\,\mu(\phi)\left(\nabla^2 v_r - \frac{v_r}{r^2}\right) + \frac{1}{We}f_r$$

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r} = 0$$

Laplacian operator | curvature

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} \qquad \kappa = \kappa_{2d} + \frac{1}{R} = \kappa_{2d} + \frac{\sin(\theta)}{r}$$

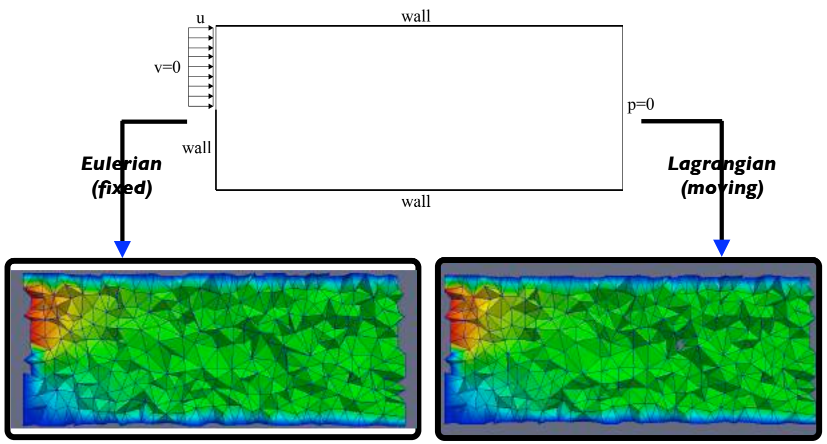
FINITE ELEMENT METHOD

PDE	weak form	ODE	linear system	approximated solution
Governing equations	Galerkin Method	Ordinary Differential Equations	Ax=b	u,v,w,p and T

Code's features:

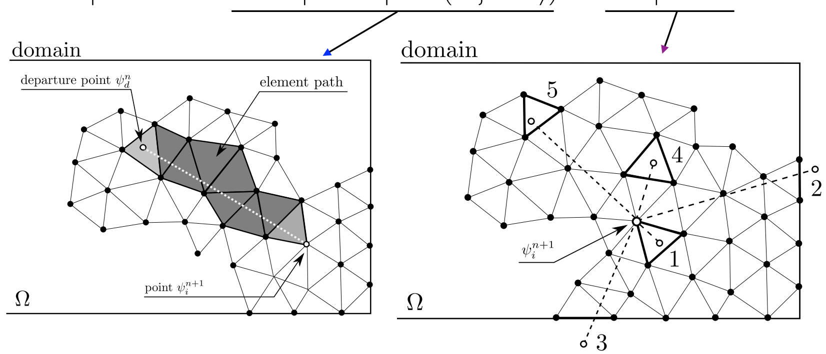
- pressure, diffusive terms → Galerkin method
- convective terms → ALE and SL methods
- time discretization → 1st. order forward difference
- linear systems → Projection method - LU
- surface tension → Geometric

EULERIAN - LAGRANGIAN



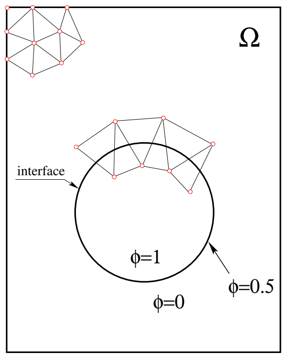
SEMI-LAGRANGIAN

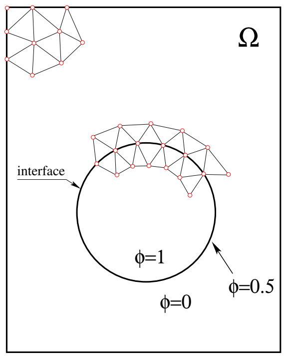
- compute advection using fixed mesh;
- discretization of material derivative: $\frac{D\psi}{Dt} = \frac{\psi^{n+1} - \psi^n}{\Delta t}$
- in ALE context: compute difference between flow field and node motion;
- 2-steps calculation: find departure point (trajectory) and interpolation.



INTERFACE DEFINITION

- Eulerian approach: (fixed mesh)
- Lagrangian approach: (moving mesh)





SURFACE TENSION

$$\mathbf{f} = \sigma\kappa\mathbf{n}\delta$$

continuum surface force model
Brackbill and Kothe (1992)

σ : surface tension coefficient

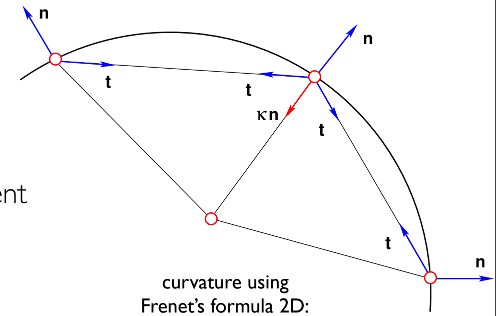
κ : curvature

δ : Dirac delta function

$\mathbf{n}$: normal vector

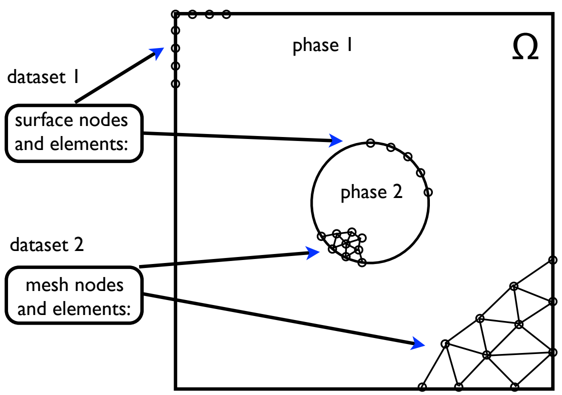
$\mathbf{t}$: tangent vector

ϕ : marker function (Heaviside)

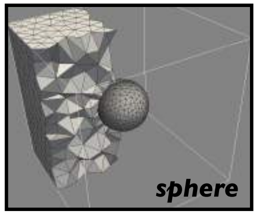


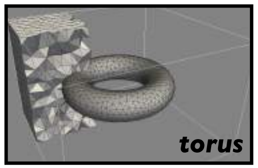
curvature using Frenet's formula 2D:

MESH STORAGE

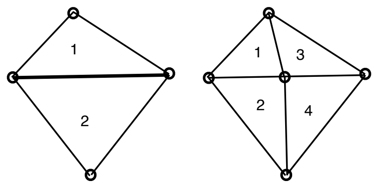


Examples:

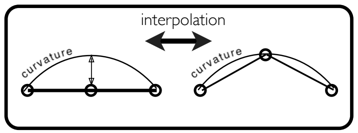




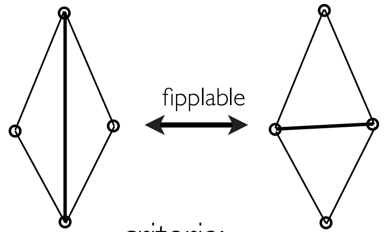
INSERTION



2D view:



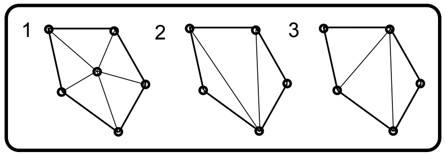
FLIPPING



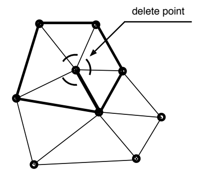
criteria:

aspect ratios, curvature, area and circumcenter

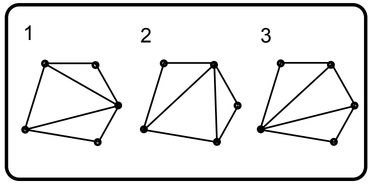
example:



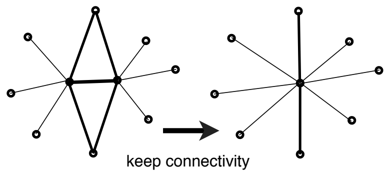
DELETION



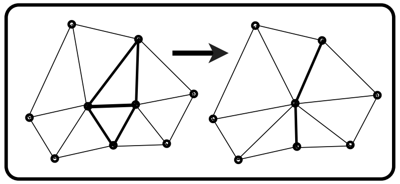
options:



CONTRACTION



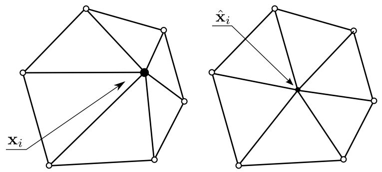
example:



NODES MOTION

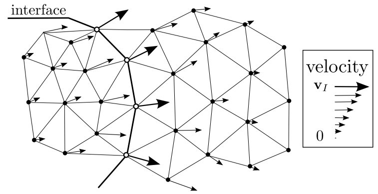
coordinates:

$$\hat{\mathbf{v}}_{e_i} = \frac{\sum_{i \in N_1(j)} e_{ij}^{-1}(\mathbf{x}_j - \mathbf{x}_i)}{dt}$$



velocities:

$$\hat{\mathbf{v}}_{v_i} = \frac{1}{n} \sum_{j \in N_1(j)} \mathbf{v}_j$$



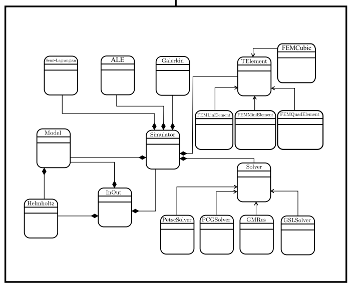
Proposed scheme:

$$\hat{\mathbf{v}}(\mathbf{x}) = \begin{cases} c_1\mathbf{v} + c_2\mathbf{v_v} + c_3\mathbf{v_e} & \text{if } \mathbf{x} \text{ does not belong to the interface} \\ \mathbf{v} - d_1(\mathbf{v}\cdot\mathbf{t})\mathbf{t} + d_2(\mathbf{v_e}\cdot\mathbf{t})\mathbf{t} & \text{if } \mathbf{x} \text{ belongs to the interface} \end{cases}$$

PYTHON API

Python3 API

C++



- step.py
- vortex.py
- stepALE.py
- poiseuilleAxi.py

- risingBubble.py
- risingBubbleTaylor.py
- sessileDrop.py
- oscillatingDrop.py
- micro.py
- microAxi.py
- risingBubbleAxi.py
- risingBubbleTaylorAxi.py

SCRIPT STRUCTURE

Python3 API

- simulation parameters
- mesh velocity
- linear system solver

- python procedures for copying and saving files

- Model constructor
- Simulator initialization

- for loop of ODE (time)

- remeshing
- interpolation new mesh

- stepALE() // convective term
- setDt() // set dt based on cfl
- printSimulationReport()
- movePoints() // move nodes
- setRHS() // set right hand side vector
- setUncoupledBC() // apply B.C.
- setGravity() // set gravity vector
- setInterface() // set interface force vector
- setUncoupled() // solve linear system
- saveMesh() // save mesh in Gmsh format
- saveVTK() // save VTK for preview
- saveSol() // save solution in binary
- saveOldData() // save solution vectors
- timeStep() // iterate in time

SOLUTION PROCEDURE

- Departure parameters $(\mathbf{v}_h^n, p_h^n)$ on mesh $\mathbf{x}_h^n$

1. Compute mesh velocities $\hat{\mathbf{v}}_h(\mathbf{x})$
2. Calculate time step Δt based on defined CFL
3. Move mesh points to new position: $\mathbf{x}_h^{n+1} = \mathbf{x}_h^n + \Delta t \hat{\mathbf{v}}_\mathbf{h}(\mathbf{x})$
4. Solve ALE N-S linear system for $(\mathbf{v}_h^{n+1}, p_h^{n+1})$
5. Perform mesh operations (deletions, insertions, flippings etc.)
6. Generate new mesh: $\mathbf{x}_h^{n+1} \longrightarrow \mathbf{x}_{\tilde{h}}^{n+1}$
7. Interpolate solution to the new mesh: $(\mathbf{v}_h^{n+1}, p_h^{n+1}) \longrightarrow (\mathbf{v}_{\tilde{h}}^{n+1}, p_{\tilde{h}}^{n+1})$

HOW TO RUN

start conda env
- open terminal
- sa fem

check 1st test case
- terminal
- cd $HOME/projects/python/femSIM2d
- python3 step.py

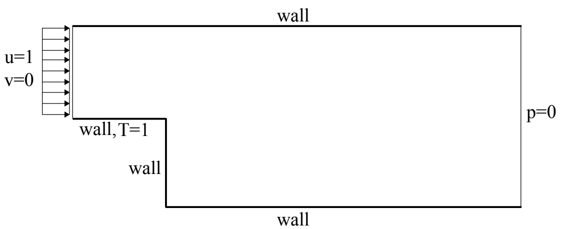
visualize 1st test case
- open paraview
- click to open file and point to
- $HOME/projects/python/femSIM2d/step

2D TESTCASES

Backward facing step

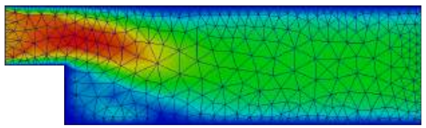
stepALE.py

$Re = 1000, Sc = 2000, \mu = 1, \rho = 1$

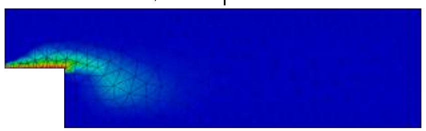


Mesh parameters:
\# Lagrangian nodes
$c1 = \{0.1, 0.0, -0.1\}$
\# Interface velocity smoothing
$c2 = \{0.0\}$
\# Laplacian smoothing
$c3 = \{2.0; 0.0, 0.1\}$

time = 37, velocity field



time = 37, temperature field

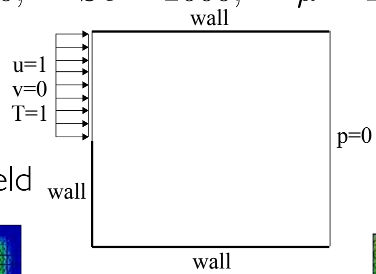


2D TESTCASES

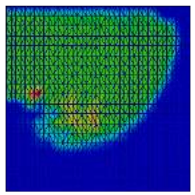
Backward facing step

step.py

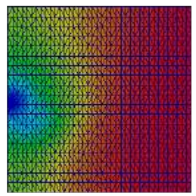
$Re = 10000, \quad Sc = 2000, \quad \mu = 1, \quad \rho = 1$



time = 20,
temperature field



time step = 5,
pressure field



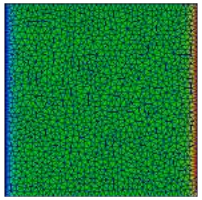
2D TESTCASES

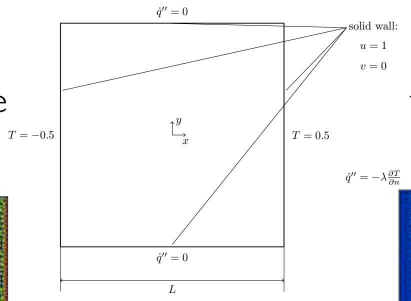
cavity with different temperature

cavity.py

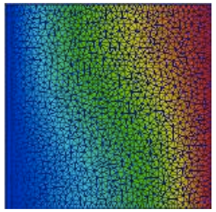
$$Re = \sqrt{1000}, Sc = 1, \frac{\rho_{in}}{\rho_{out}} = 1, \frac{\mu_{in}}{\mu_{out}} = 1$$

temperature iter=0





temperature iter=100



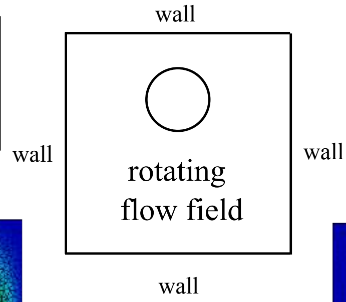
2D TESTCASES

drop under rotating flow

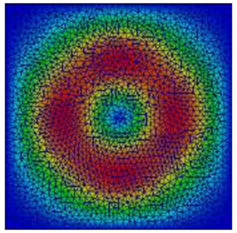
vortex.py

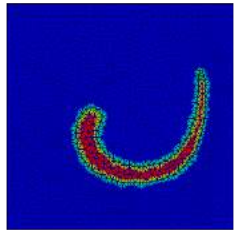
flow field

$v_x = -\sin^2(\pi x)\sin(2\pi y)$
$v_y = \sin^2(\pi y)\sin(2\pi x)$



Play with mesh parameters c1,c2,c3,d1 and d2



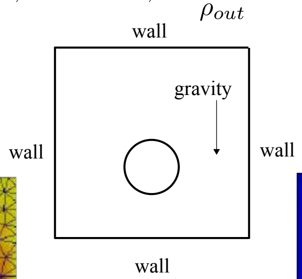


2D TESTCASES

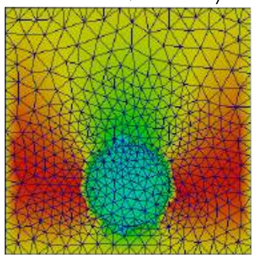
sessile drop

sessileDrop.py

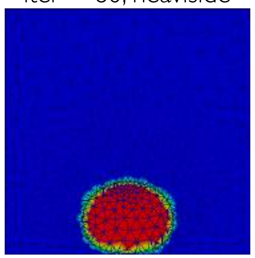
$$Re = 20, \quad We = 20, \quad Fr = 1, \quad \frac{\rho_{in}}{\rho_{out}} = 1000, \quad \frac{\mu_{in}}{\mu_{out}} = 1.111$$



iter = 10; velocity



iter = 60; heaviside

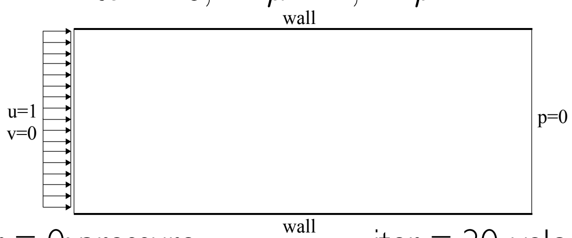


2D TESTCASES

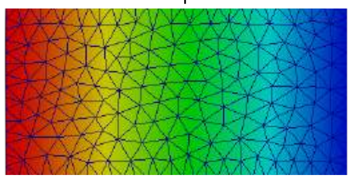
Poiseuille

poiseuille.py

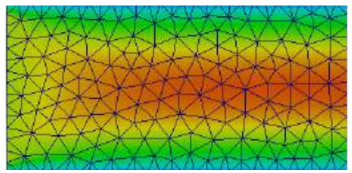
$$Re = 20, \quad \mu = 1, \quad \rho = 1$$



iter = 0; pressure



iter = 20, velocity



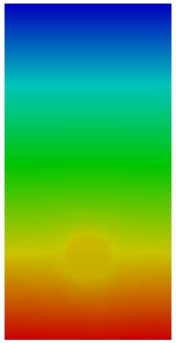
2D TESTCASES

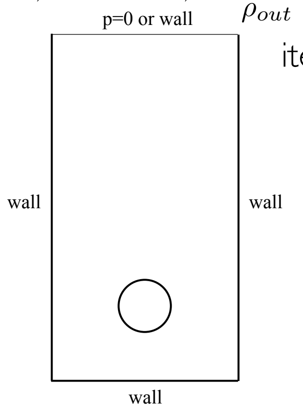
Rising bubble

risingBubble.py

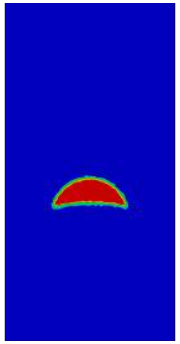
$$Re = 100, \quad We = 10, \quad Fr = 1, \quad \frac{\rho_{in}}{\rho_{out}} = 10, \quad \frac{\mu_{in}}{\mu_{out}} = 10$$

iter = 0; pressure





iter = 270; heavisde

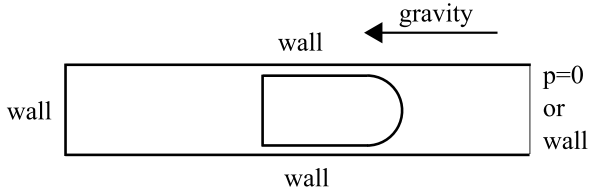


2D TESTCASES

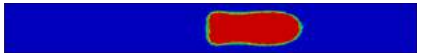
Rising of Taylor bubble - *moving frame*

risingBubbleTaylor.py

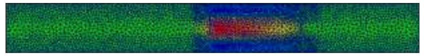
$$Re = 100, \quad We = 10, \quad Fr = 1, \quad \frac{\rho_{in}}{\rho_{out}} = 10, \quad \frac{\mu_{in}}{\mu_{out}} = 10$$



iter = 110; heaviside



iter = 110; velocity

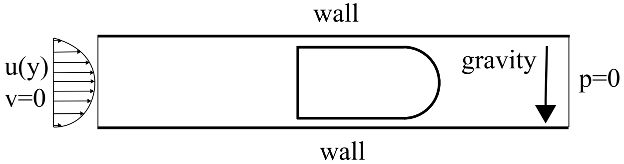


2D TESTCASES

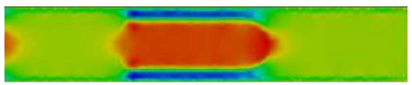
bubble in microchannel - *moving frame*

micro.py

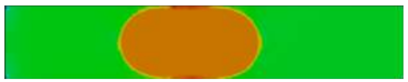
$$Re = 576.24, \quad We = 1.162, \quad Fr = 10.096, \quad \frac{\rho_{in}}{\rho_{out}} = 1509.39, \quad \frac{\mu_{in}}{\mu_{out}} = 180.169$$



iter = 05; velocity field



iter = 850; pressure

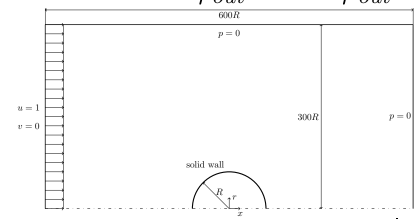


AXI TESTCASES

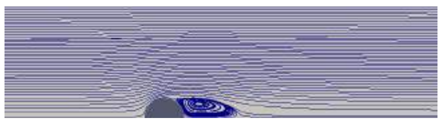
Flow around sphere

sphereAxi.py

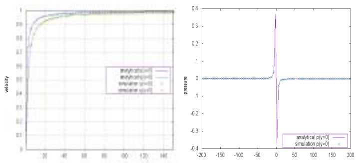
$$Re = 0.00001, \quad \frac{\rho_{in}}{\rho_{out}} = 1 \quad \frac{\mu_{in}}{\mu_{out}} = 1$$



high Re



low Re

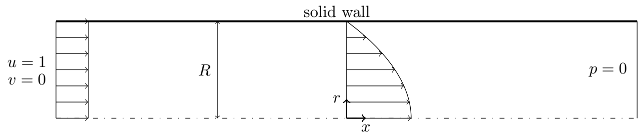


AXI TESTCASES

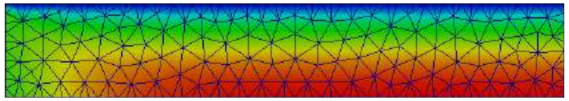
Poiseuille flow

poiseiulleAxi.py

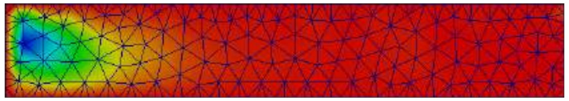
$$Re = 20, \quad \frac{\rho_{in}}{\rho_{out}} = 1, \quad \frac{\mu_{in}}{\mu_{out}} = 1$$



v_x velocity



v_r velocity

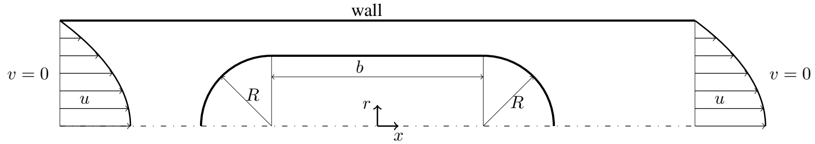


AXI TESTCASES

Isolated air bubble in glycerol solution through microchannel

microAxi.py

$$Re = 0.0128552, \quad We = 0.00127691, \quad \frac{\rho_{in}}{\rho_{out}} = 9.632 \cdot 10^{-4}, \quad \frac{\mu_{in}}{\mu_{out}} = 3.455 \cdot 10^{-5}$$



Initial mesh (1630 vertices), final mesh (14718 vertices)

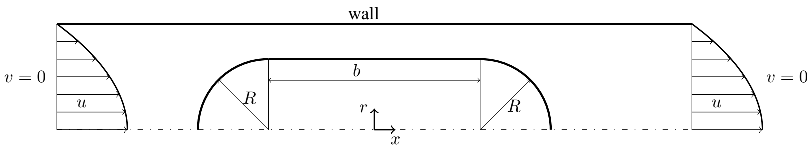
* **Khodaparast, S.; Magnini, M.; Borhani, N.; Thome, J.R.** Dynamics of isolated confined air bubbles in liquid flows through circular microchannels.- Microfluidics and Nanofluidics., **19:** 209-234 (2015)

AXI TESTCASES

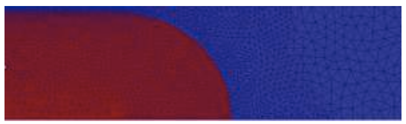
Isolated air bubble in water through microchannel

microAxi.py

$$Re = 140.93, \quad We = 0.4122, \quad \frac{\rho_{in}}{\rho_{out}} = 1.2076 \cdot 10^{-3}, \quad \frac{\mu_{in}}{\mu_{out}} = 2.159 \cdot 10^{-2}$$



mesh



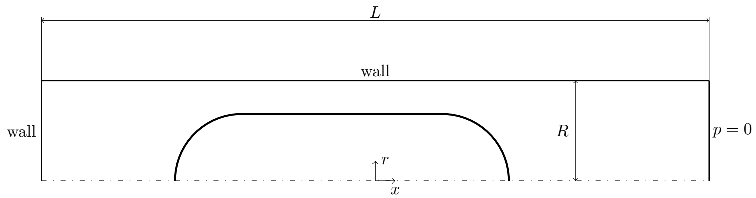
streamlines

AXI TESTCASES

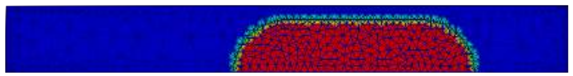
rising of isolated taylor bubble in microchannel

risingBubbleTaylorAxi.py

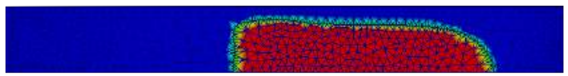
$$Re = 159.054, \quad We = 40, \quad Fr = 1, \quad \frac{\rho_{in}}{\rho_{out}} = 1038.37, \quad \frac{\mu_{in}}{\mu_{out}} = 2275.28$$



heaviside, iter=0



heaviside, iter=180

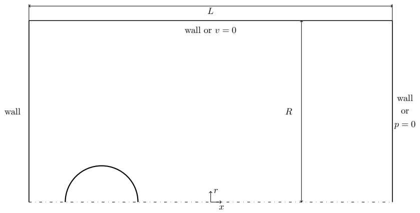


AXI TESTCASES

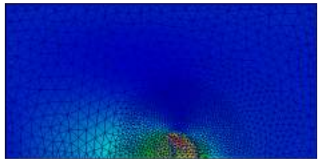
rising of air bubble
in sugar solution

risingBubbleAxi.py

$$Re = 13.84, \quad We = 115.662, \quad Fr = 1, \quad \frac{\rho_{in}}{\rho_{out}} = 1102.04, \quad \frac{\mu_{in}}{\mu_{out}} = 71910.1$$



v_x velocity



v_r velocity