Level Set Methods for Two-Phase Flows with FEM

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Importance of Multiphase Flow Simulations

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Importance of Multiphase Flow Simulations

- Multiphase flow simulations are fundamental tools in a wide range of industrial applications such as liquid phase sintering and inkjet printing
- Replacing expensive and complicated laboratory experiments
- **Two-phase flow** is a branch of multiphase flows
    - Flows including two incompressible fluids that do not mix, such as oil and water, are called two-phase flows

Introduction

Numerical Aspect and Goal

- An efficient and accurate implementation of the numerical methods for two-phase flows is not trivial

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Numerical Aspect and Goal

- An efficient and accurate implementation of the numerical methods for two-phase flows is not trivial
- The aim of the project is to implement two different **level set methods** and analyse and compare the numerical results

Introduction

Discretization : FEM versus FVM

- Flow simulations are usually discretized using the Finite Volume Method (FVM) or Finite Element Method (FEM) in space along with finite difference method (FDM) for time discretization

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- **FEM** could be easily improved in giving high order accuracy with more computational cost, whereas it becomes complex and difficult to solve in high order accuracy in the other methods
- Therefore, we use the FEM for the spatial discretization and the FDM for the temporal discretization

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- After choosing the type of the implicit function, the domain values that give $\phi(\mathbf{x}) = 0$ represent the interface between the two incompressible fluids

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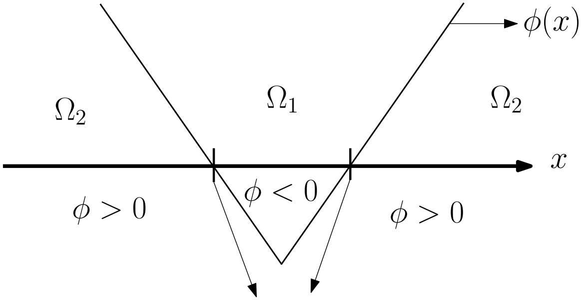
- Level Set Method = Level Set Function + Reinitialization

Level Set Methods

Level Set Functions



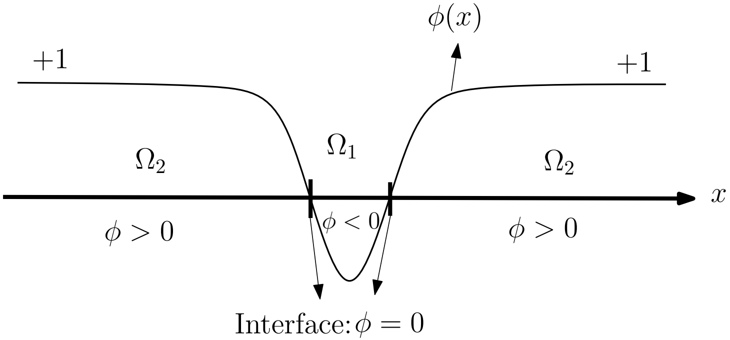
Interface: $\phi = 0$

Standard level set function:

$$\phi(\mathbf{x}) = d(\mathbf{x}) - R$$

Level Set Methods

Level Set Functions



Conservative level set function:

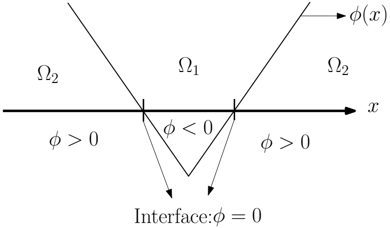
$$\phi(\mathbf{x}) = \tanh(d(\mathbf{x}) - R)$$

Level Set Methods

Reinitialization

Reinitialization : Standard Level Set Function

$$\underbrace{\frac{\partial \phi}{\partial \tau}}_{\text{Mass}} + \underbrace{S_\epsilon(\phi_0)(|\nabla \phi| - 1)}_{\text{Smoothing}} = 0$$



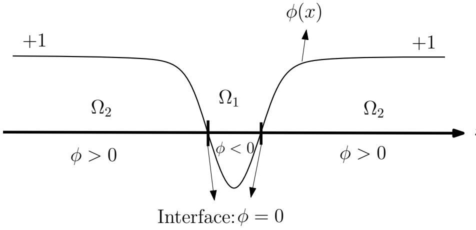
Level Set Methods

Reinitialization

Reinitialization : Conservative Level Set Function

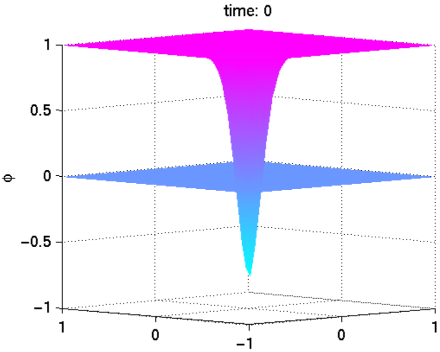
$$\underbrace{\frac{\partial \phi}{\partial \tau}}_{\text{Mass}} + \underbrace{\nabla \cdot (\mathbf{n}(1-\phi^2))}_{\text{Compressing}}$$

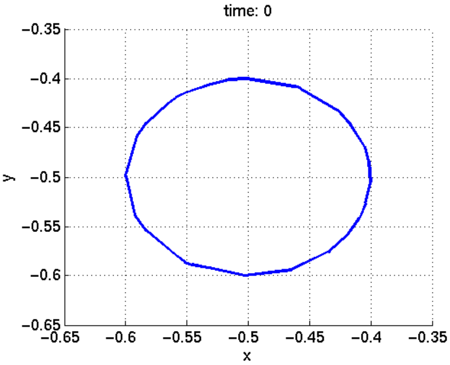
$$- \underbrace{\nabla \cdot (\mathbf{n}\varepsilon \nabla \phi \cdot \mathbf{n})}_{\text{Diffusing}} = 0$$



Level Set Methods

Initial position in our case





Conservative level set function in 2D

Level Set Methods

How a Level Set Function moves

The convection equation:

$$\underbrace{\frac{\partial \phi}{\partial t}}_{\text{Mass}} + \underbrace{\mathbf{u} \cdot \nabla \phi}_{\text{Movement}} = 0$$

where $\mathbf{u}$ is the fluid vector.

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Why to use a Level Set Method?

Advantages of level set methods:

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Discretization is straightforward:

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  1. Stabilization problem
  2. Resolution problem
  3. Necessity of Reinitialization
  4. Parameters (arises from solving the previous problems)

Level Set Methods

Discretizations: Stabilization Problem

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Level Set Methods

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Level Set Methods

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  - **Problem**: Standard finite element approximation causes oscillations due to the high sensitivity of big values of the term $\nabla\phi$
  - **Solution**: Instead, it is approximated with Galerkin Least Squares (GLS) finite element and the following stabilization parameter is introduced:
    $\delta = ch/\|\mathbf{u}\|_{L^\infty(\Omega)}$
    where h is mesh size, c is a constant to be chosen, $\mathbf{u}$ is the fluid velocity and Ω is the given space domain

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  - **Solution**: The GLS method gives us a parameter to play around, we could modify it accordingly

Level Set Methods

Discretizations: Resolution Problem

Discretization gives number of nodes which might not represent the solution in a correct way

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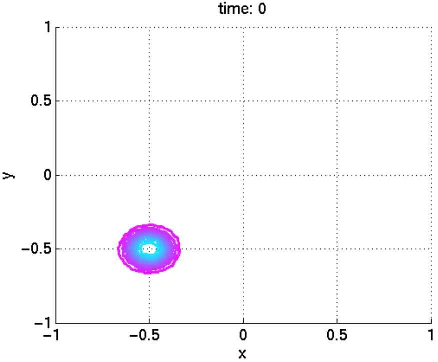
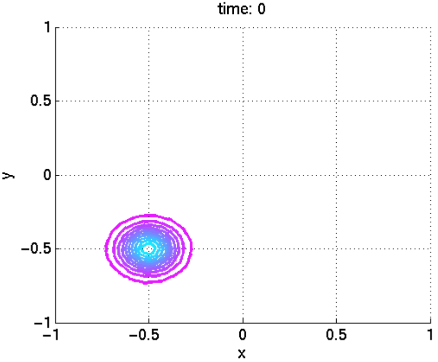
- **Problem**: The conservative level set function might be too steep so that it can cause oscillations
- **Solution**: The function can be formulated as $\phi(\mathbf{x}) = \tanh((d(\mathbf{x}) - R)/\epsilon h)$, where ϵ is an adjustment for the steepness of the function

Level Set Methods

Discretizations: Resolution Problem (only for the conservative level set function)

Example:





. $\epsilon = 1$ $\epsilon = 2$

Conservative level set function in 2D in contour

Level Set Methods

Discretizations: Necessity of Reinitialization

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Level Set Methods

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Level Set Methods

Discretizations: Necessity of Reinitialization

- **Problem**: The shape of the *interface* deforms in the numerical solution.
- **Solution**: Additional numerical method to fix: Reinitialization
  - The reinitialization for the both level set functions are discretized in FEM with linear hat function and backward Euler method (FDM)
  - Since it is an additional method, this method is iterated **twice** in each movement

Level Set Methods

Discretizations: Full Discretizations

- Full discretization for the convection equation:

$$(2M + \Delta t(C + \delta SD))\xi^{n+1} = (2M - \Delta t(C + \delta SD))\xi^{n}$$

where SD is the streamline-diffusion matrix.

Level Set Methods

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  where SD is the streamline-diffusion matrix.

- Full discretization for the reinitialization for the standard level set function:

$$M\xi^{n+1} = M\xi^{n} + \Delta\tau(S_{\varepsilon}(\phi_0)(1 - |\nabla\tilde{\phi}|))$$

  where $\Delta\tau$ is pseudo-time step, $\tilde{\phi}$ is the previous solution.

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Discretizations: Full Discretizations

- Full discretization for the convection equation:

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  where $\Delta\tau$ is pseduo-time step, $\tilde{\phi}$ is the previous solution.
- Full discretization for the reinitialization for the conservative level set function:

$$(M + \Delta\tau\varepsilon A)\xi^{n+1} = M\xi^{n} + \Delta\tau(2\tilde{\phi}|\nabla\tilde{\phi}| - (1 - \tilde{\phi}^2)\frac{\Delta\tilde{\phi}}{|\nabla\tilde{\phi}|})$$

  where ε is diffusion parameter.

Level Set Methods

Discretizations: A new problem: Parameters

Number of parameters increases to 6 from 2, which makes it difficult to control and obtain the best result

Name	**Symbol**	**Feature and Dependency**
Mesh Size	h	The smaller h, the higher resolution
Time Step	Δt	Proportional to the number of time steps for a fixed time in the simulation
Stability Parameter Constant	c	Stabilization for the convection equation using the FEM, it does not depend on h, but the stability parameter δ does
Pseudo-Time Step	$\Delta\tau$	Pseudo time step for the reinitialization, depends on Δt
Number of Reinitialization Iterations	$iter$	Adjustment to the reinitialization, mainly depends on $\Delta\tau$ but may also depend on Δt
Diffusion Parameter	ε	Smoother for the numerical solution of the conservative level set function, may depend on h

Level Set Methods

Initial and Boundary Conditions

- *Initial Condition*: Initial level set function value with the centre of the circle, $\mathbf{x}_c$, and the radius, R, in 2D to give a unique solution

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-

Level Set Function	Standard	Conservative
$\mathbf{x}_c$	$(-0.5, -0.5)^T$	$(-0.5, -0.5)^T$
R	0.1	0.1
BCs	Fixed, moving with $\mathbf{x}_c$	Completely fixed

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Numerical Experiments and Results: Experiment Case

What is Experiment Case?

We want to test how well the level set methods work. For this:

- We must know the analytical solution when the simulation finishes at time T

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We want to test how well the level set methods work. For this:

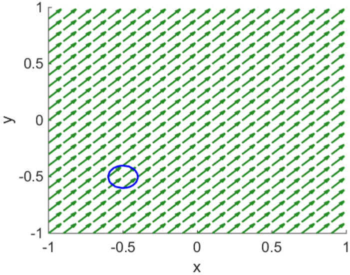
- We must know the analytical solution when the simulation finishes at time T
- The fluid vector $\mathbf{u}$ must be constant and uniform

Numerical Experiments and Results: Experiment Case

Setting up the numerical experiment

Experiment values:

- The grid domain is $[-1, 1] \times [-1, 1]$.



Numerical Experiments and Results: Experiment Case

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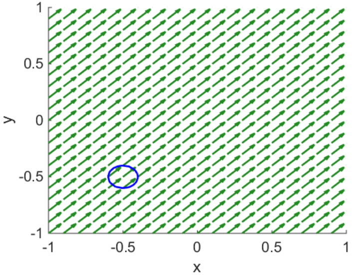
- The grid domain is $[-1, 1] \times [-1, 1]$.
- The fluid vector, $\mathbf{u}(\mathbf{x}) = \begin{pmatrix} u_x(\mathbf{x}) \\ u_y(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} 0.05 \\ 0.05 \end{pmatrix}$



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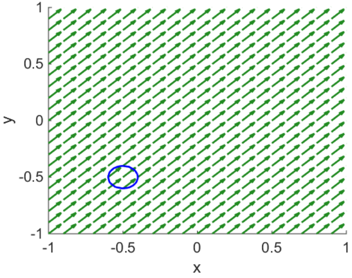
- The circle is at the centre $\mathbf{x}_c = (-0.5, -0.5)^T$ with $R = 0.1$



Numerical Experiments and Results: Experiment Case

Setting up the numerical experiment

Parameters for the level set methods:

Level Set Method	Standard	Conservative
h	varies as 0.1, 0.05, and 0.025	varies as 0.1, 0.05, and 0.025
Δt	0.01	0.01
c	0.5	0.5
$\Delta\tau$	$0.01\Delta t$	$0.001\Delta t$
$iter$	2	2
ε	Not applicable	0.001

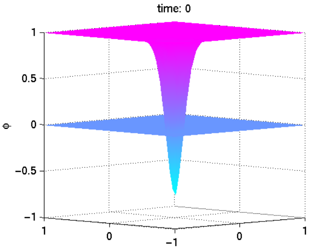
Simulation stops when $T = 1.00$

Numerical Experiments and Results: Experiment Case

Error Measurement

We consider two different types of error:

- The level set function error

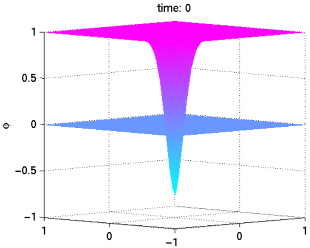


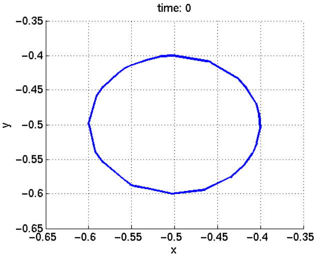
Numerical Experiments and Results: Experiment Case

Error Measurement

We consider two different types of error:

- The level set function error
- The area error (more important)





Numerical Experiments and Results: Experiment Case

Results

We have identified three different effects:

1. Effect of the stability constant parameter c

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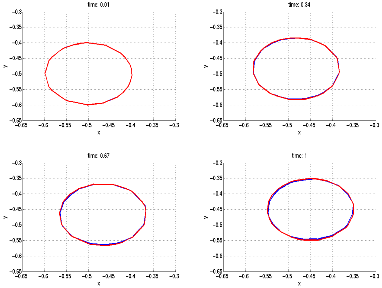
1. Effect of the stability constant parameter c
2. Effect of the position of the interface
3. Effect of the reinitialization

Numerical Experiments and Results: Experiment Case

Results : Effect of the stability constant parameter c

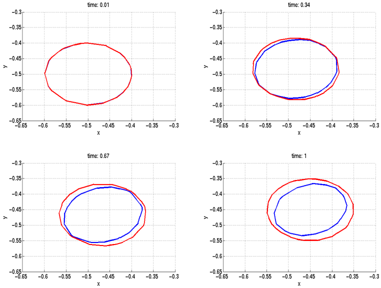
The ODE (semi-discretized) form of the new convection equation:

$$\dot{\xi}(t) = -M^{-1}(C + \delta SD)\xi(t)$$



Zero contours for $c = 0.05$

$\lambda_{max} = +0.64822$



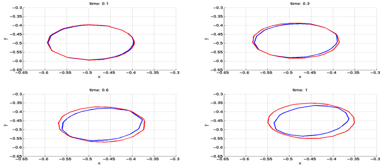
Zero contours for $c = 0.5$

$\lambda_{max} = +1.3641 \times 10^{-15}$

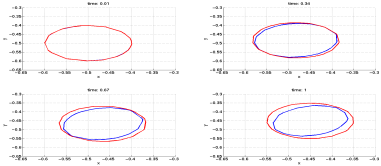
The plots are the standard level set function when $h = 0.05$ without reinitialization

Numerical Experiments and Results: Experiment Case

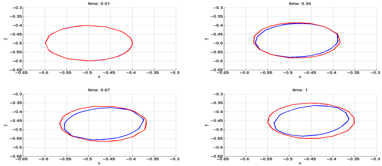
Results : Effect of the position of the interface



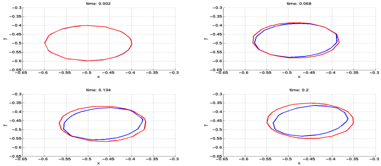
$\mathbf{u} = (0.05, 0.05)^T$, $\Delta t = 0.1$, and $T = 1.0$



$\mathbf{u} = (0.05, 0.05)^T$, $\Delta t = 0.01$, and $T = 1.00$



$\mathbf{u} = (0.05, 0.05)^T$, $\Delta t = 0.001$, and $T = 1.000$



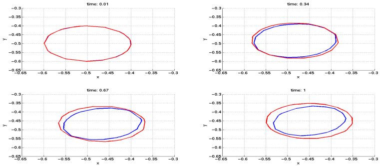
$\mathbf{u} = (0.25, 0.25)^T$, $\Delta t = 0.001$, and $T = 0.200$

The plots are the conservative level set function when $h = 0.05$ without reinitialization

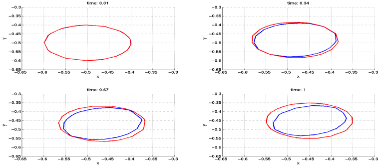
Numerical Experiments and Results: Experiment Case

Results : Effect of the reinitialization

Different results for the different level set function for $h = 0.05$



Standard level set function WITHOUT reinitialization



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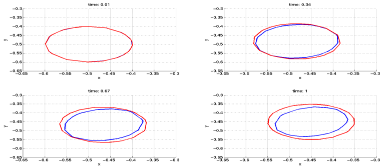

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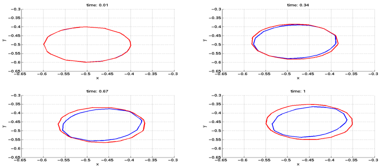
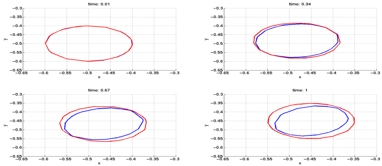
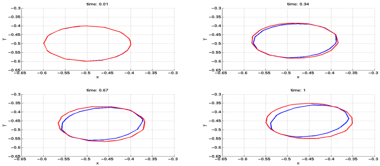


Conservative level set function WITHOUT reinitialization



Standard level set function WITH reinitialization

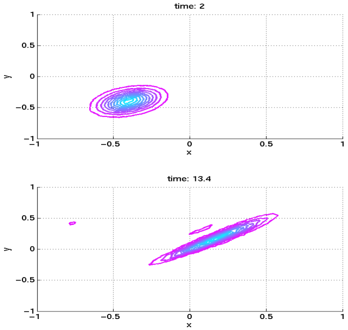


Conservative level set function WITH reinitialization

Numerical Experiments and Results: Experiment Case

Results : Effect of the Reinitialization

The reinitialization acts as an exerted force on the level set function. And indeed, new arbitrary contours occurs after a long time in the conservative level set method for $c = 0.5$, which is a sign for **instability**.

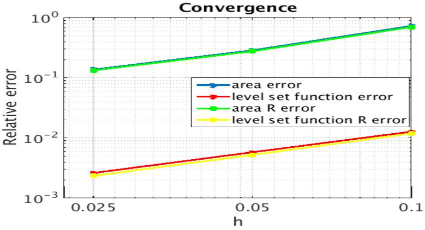


The plots are the conservative level set function when $h = 0.05$

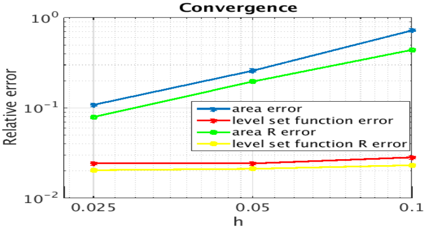
Numerical Experiments and Results: Experiment Case

Results : Grid Convergence and Convergence Rates

Here Δt is chosen such as $\Delta t / h = 0.1$



Standard level set method



Conservative level set method

Level set function	Standard		Conservative	
Reinitialization included?	NO	YES	NO	YES
Relative level set function error	1.1436	1.1718	0.1086	0.1039
Relative area error	1.2065	1.1973	1.3701	1.2362

Simulation terminates when $T = 1.00$

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Fluid Mechanics

Why to use Fluid Mechanics?

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- We want to test the level set methods on a more complicated system, which is called *benchmark case*
- We find the numerical solution for the fluid velocity, $\mathbf{u}$
- The solution follows strictly as in Larson and Bengzon's book: *The Finite Element Method, Theory, Implementation, and Applications*

Fluid Mechanics

Mathematical Model

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$$\Delta \mathbf{u} + \nabla p = \mathbf{f}, \quad \text{in } \Omega$$
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- Note that since there is only ∇p in the equations, the pressure needs to have a zero mean value (the hydrostatic pressure level):

$$\frac{\int\limits_{\Omega} p \, \mathrm{d}\Omega}{|\Omega|} = 0$$

Fluid Mechanics

Discretization

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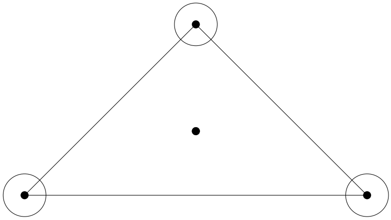
Fluid Mechanics

Discretization

- Since we need to solve for the velocity $\mathbf{u}$ and pressure p, we create two different test functions in Hilbert and L^2-norm spaces, respectively
- Moreover, the MINI element provides the pair solution $(\mathbf{u}, p)$ in solving the resulting form of FEM from the weak forms due to being the simplest inf-sup stable element and easy to implement.



A triangulation of MINI element in 2D where • represents velocity and ◯ represents pressure at the given nodes

Fluid Mechanics

Discretization

The final discretization is:

$$\begin{bmatrix} A & 0 & B_x & 0 \\ 0 & A & B_y & 0 \\ B_x^T & B_y^T & 0 & a \\ 0 & 0 & a^T & 0 \end{bmatrix} \begin{bmatrix} u_x \\ u_y \\ p \\ \mu \end{bmatrix} = \begin{bmatrix} b_x \\ b_y \\ 0 \\ 0 \end{bmatrix}$$

where A is the stiffness matrix, B_x and B_y are divergence matrices, a is the operator from the hydrostatic pressure level, b_x and b_y are the load vectors, μ is a Lagrangian multiplier and the numerical velocity $\mathbf{u} = (u_x, u_y)^T$ (taken) and numerical pressure p (disregarded)

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Numerical Experiments and Results: Benchmark Case

What is Benchmark Case?

We want to test how well the level set methods work *in a complicated system*. For this:

- We do not know the analytical solution (for the level set function) when the simulation finishes at time T

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What is Benchmark Case?

We want to test how well the level set methods work *in a complicated system*. For this:

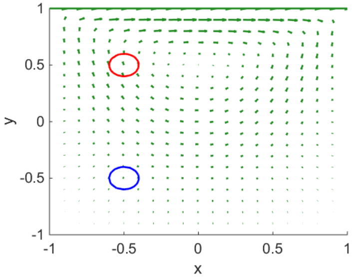
- We do not know the analytical solution (for the level set function) when the simulation finishes at time T
- The fluid vector $\mathbf{u}$ is already complicated from the fluid mechanics

Numerical Experiments and Results: Benchmark Case

Setting up the numerical experiment

Experiment values:

- The grid domain is $[-1, 1] \times [-1, 1]$.



Numerical Experiments and Results: Benchmark Case

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- The grid domain is $[-1, 1] \times [-1, 1]$.
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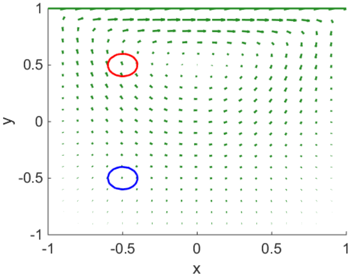

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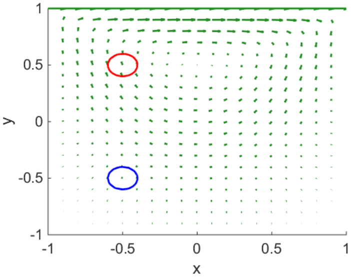
- Since the velocity field varies, we consider two different initial positions of the interface



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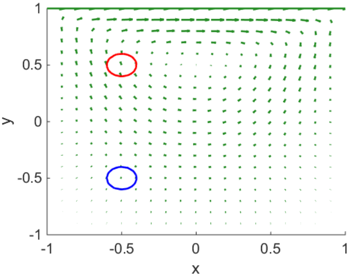
    - **Upper Position**: The circle is at the centre $\mathbf{x}_c = (-0.5, 0.5)^T$ with $R = 0.1$ (red)



Numerical Experiments and Results: Benchmark Case

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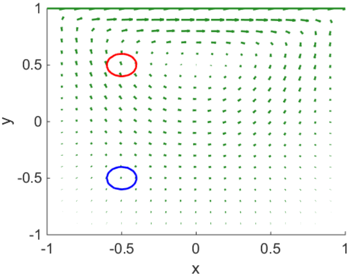
    - **Upper Position**: The circle is at the centre $\mathbf{x}_c = (-0.5, 0.5)^T$ with $R = 0.1$ (red)
    - **Lower Position**: The circle is at the centre $\mathbf{x}_c = (-0.5, -0.5)^T$ with $R = 0.1$ (blue)



Numerical Experiments and Results: Benchmark Case

Setting up the numerical experiment

Parameters for the level set methods:

	Benchmark case	
Level Set Method	Standard	Conservative
h	varies as 0.1, 0.05, and 0.025	varies as 0.1, 0.05, and 0.025
Δt	0.01	0.01
c	1.0	1.0
$\Delta \tau$	$0.01\Delta t$	$0.001\Delta t$
iter	2	2
ε	Not applicable	0.001

Simulation stops when $T = 1.00$

Numerical Experiments and Results: Benchmark Case

Error Measurement

We consider only one type of error

- Since we do not know the analytical solution of the level set function at time T, there is no level set function error

Numerical Experiments and Results: Benchmark Case

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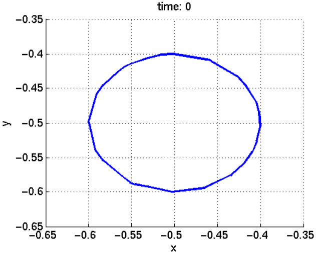
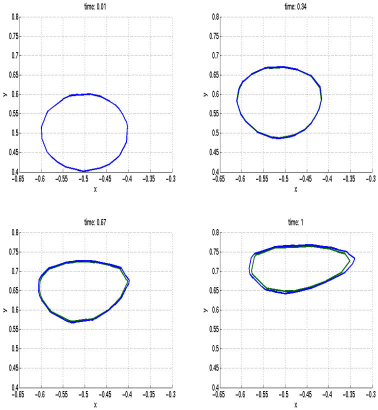
- Since we do not know the analytical solution of the level set function at time T, there is no level set function error
- We know the analytical area from the initial position, πR^2, so we can calculate the area error (more important)



Numerical Experiments and Results: Benchmark Case

Results: Upper Position

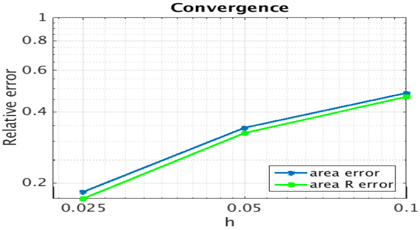


The plots are the conservative level set function when $h = 0.05$

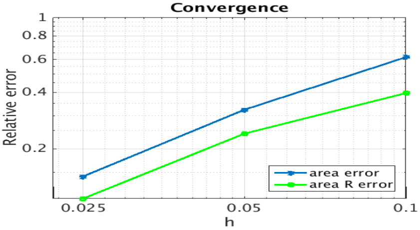
Numerical Experiments and Results: Benchmark Case

Results: Upper Position : Grid Convergence and Convergence Rates

Here Δt is chosen such as $\Delta t/h = 0.1$



Standard level set method



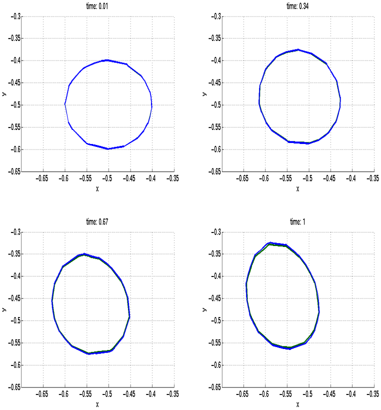
Conservative level set method

Level set function	Standard		Conservative	
Reinitialization included?	NO	YES	NO	YES
Relative area error	0.6951	0.7152	1.0557	0.9343

Simulation terminates when $T = 1.00$

Numerical Experiments and Results: Benchmark Case

Results: Lower Position

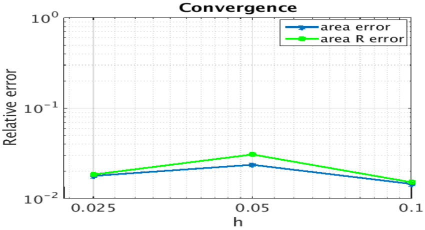


The plots are the conservative level set function when $h = 0.05$

Numerical Experiments and Results: Benchmark Case

Results: Lower Position : Grid Convergence and Convergence Rates

Here Δt is chosen such as $\Delta t/h = 0.1$



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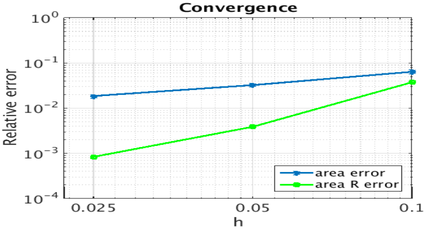

Conservative level set method

Level set function	Standard		Conservative	
Reinitialization included?	NO	YES	NO	YES
Relative area error	-0.1478	-0.1418	0.8893	2.7398

Simulation terminates when $T = 1.00$

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Conclusion

Comments on stability

- The stability has to be measured carefully as it has imbalance between space stability and time stability as well as with the reinitialization

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- The stability has to be measured carefully as it has imbalance between space stability and time stability as well as with the reinitialization
- The value c significantly increases when we use it in the benchmark case comparing to the one in the experiment case

Conclusion

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- The convergence rates in the numerical results for the both experiment and benchmark cases show that reinitializations usually give a better result by reducing the errors

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- The convergence rates in the numerical results for the both experiment and benchmark cases show that reinitializations usually give a better result by reducing the errors
  - The reinitialization in the standard level set method tries to preserve as much as it can
  - The reinitialization in the conservative level set method expands the interface

Conclusion

Comments in general

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Comments in general

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- For the given values for parameters in the two level set methods, we were able to show:
  - The conservative level set function is better than the standard level function
  - The reinitialization methods give a better solution under certain conditions
- Nevertheless, they all depend on velocity field, the type of level set functions and reinitializations, boundary conditions, and parameters

Conclusion

Further Research

- Another FEM stabilization method, which is other than GLS method, in order to solve the stabilization problem in 2D (in the next slide)

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- Another FEM stabilization method, which is other than GLS method, in order to solve the stabilization problem in 2D (in the next slide)
- Different kinds of level set methods in order to find one that affects the solution in a much better way

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More on the Research

New Method : Residual based artificial viscosity method

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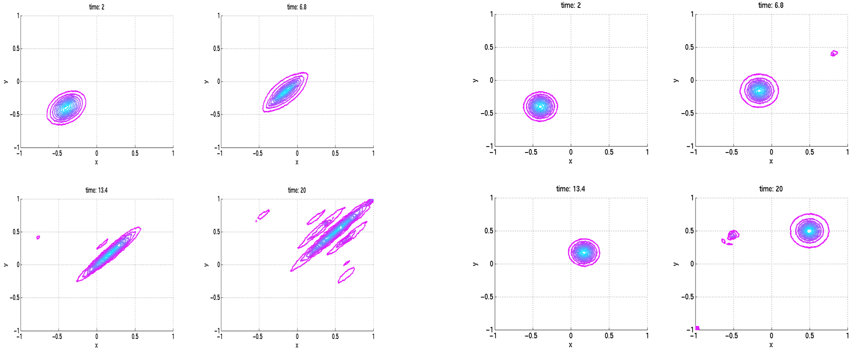
  - $\delta = ch/\|\mathbf{u}\|_{L^\infty(\Omega)} \quad \rightarrow \quad \delta = 2ch\|\mathbf{u}\|_{L^\infty(\Omega)}$
  - $c = 0.5 \quad \rightarrow \quad c = 0.03$

More on the Research

New Method : Residual based artificial viscosity method : Results



GLS method

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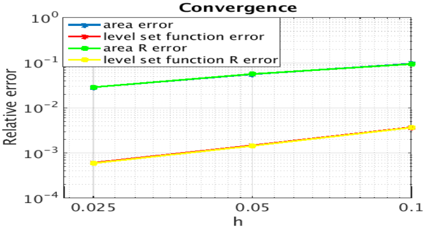
Residual based artificial viscosity method

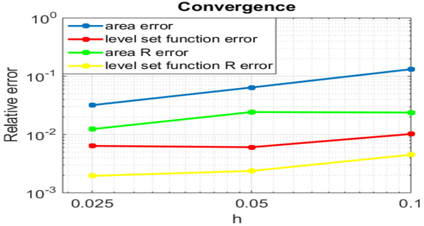
More on the Research

New Method : Residual based artificial viscosity method : Results

Here Δt is chosen such as $\Delta t/h = 0.1$



Standard level set method



Conservative level set method

Level set function	Standard		Conservative	
Reinitialization included?	NO	YES	NO	YES
Relative level set function error	1.3063	1.3158	0.3387	0.6027
Relative area error	0.8645	0.8531	1.0234	0.4744

Simulation terminates when $T = 1.00$

Questions?