# Symmetrizing multiphase flow equations for improved accuracy

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## Introduction

One common relation in modeling multiphase flow using the phase-field method is that the summation of the order parameters is equal to unity. In the present work, we aim to show the effects of this analytical relation on the results and resources when it is employed in a numerical settings. Its effects in terms of accuracy and stability of the numerical results and also the computational cost will be investigated via several numerical tests. A modified color-gradient (CG) model is the model of choice in this study. It is shown that by taking into account the summation relation of the order parameters, numerical results become unsymmetrical. Also, in some cases, it results in nonphysical interfaces. In terms of computational resources, the one-eq scheme (when one order parameter is solved through the phase-field equation and the other is obtained by the summation relation) is about 11% faster with 25% less computational memory usage than the two-eq scheme (two order parameter are determined by solving two phase-field equations). It is shown that only for a zero velocity domain the one-eq and two-eq schemes lead to the same results.

## Numerical Methods

In the phase-field context (the modified CG method), the order parameters are governed by the following phase-field formulation [1] (Subscripts $r$ and $b$ represent the *red* and *blue* fluid, respectively):

$$\frac{\partial \phi_r}{\partial t} + \boldsymbol{\nabla}.(\boldsymbol{u}\phi_r) = D\nabla^2\phi_r - D\frac{4}{\xi}\boldsymbol{\nabla}.\left[\frac{\phi_r\phi_b}{\phi_r+\phi_b}\boldsymbol{n}\right]$$
$$\frac{\partial \phi_b}{\partial t} + \boldsymbol{\nabla}.(\boldsymbol{u}\phi_b) = D\nabla^2\phi_b + D\frac{4}{\xi}\boldsymbol{\nabla}.\left[\frac{\phi_r\phi_b}{\phi_r+\phi_b}\boldsymbol{n}\right] \qquad (1)$$

where the order parameter $\phi_k$ is zero or one when the cell is without or filled with fluid $k$, respectively. The unit normal vector is $\boldsymbol{n} = \boldsymbol{\nabla}\phi/|\boldsymbol{\nabla}\phi|$ where the order parameter $\phi$ is computed based on:

$$\phi = \frac{1}{2}\left[\frac{\phi_r-\phi_b}{\phi_r+\phi_b}+1\right] \qquad (2)$$

The order parameter changes smoothly across fluid-fluid interfaces. As such, in analytical modeling we assume that the summation of the order parameters is always equal to one (summation relation):

$$\sum_k \phi_k = 1, \qquad k = r, b \qquad (3)$$

One can solve one of the two equations of (1) and compute the other order parameter based on the summation relation (3). In this case, relation (2) reduces to $\phi = \phi_r$ (assume that we solve the order parameter of the *red* fluid, as such $\phi_b = 1-\phi_r$). However, in numerical simulations, the summation relation (3) does not always hold due to dispersion errors. In the following results, we will show that by considering the summation relation (3) results are unsymmetrical and inaccurate. We therefore propose to implement a two-eq scheme, where two lattice-Boltzamnn (LB) equations are employed to recover the macroscopic interfacial evolution equations, in contrast to the one-eq scheme, where only one LB equation is employed and the order parameter of the other fluid is determined based on (3). We also use another LB for recovering the hydrodynamic properties [2,3] with the density computed through:

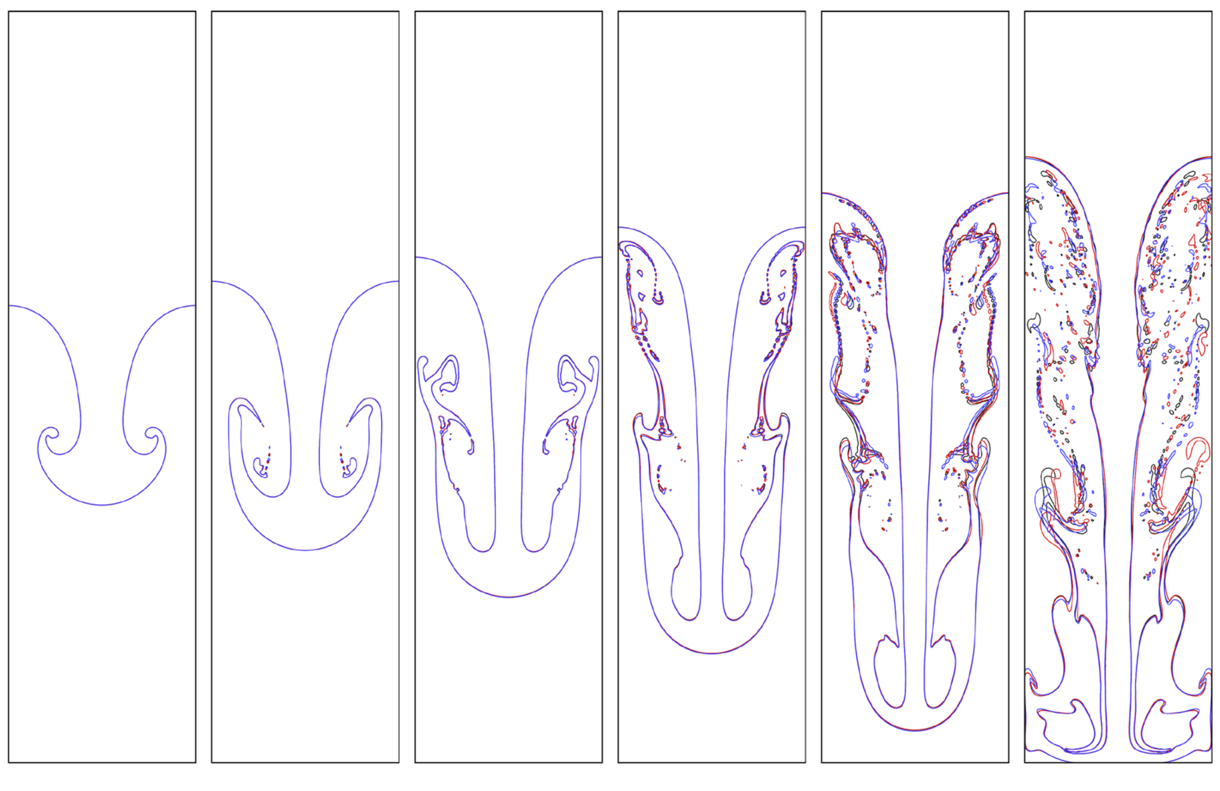
$$\rho = \phi_r\rho_r + \phi_b\rho_b$$

## Results

Different benchmarks are considered to investigate the differences between the one-eq and two-eq schemes. These two schemes are compared in terms of accuracy and computational cost. Throughout the study, interface thickness $\xi$ and the mobility $D$ are respectively determined with the Cahn number ($\mathrm{Ch} = \xi/L_0$) and the Peclet number ($\mathrm{Pe} = U_0L_0/D$).

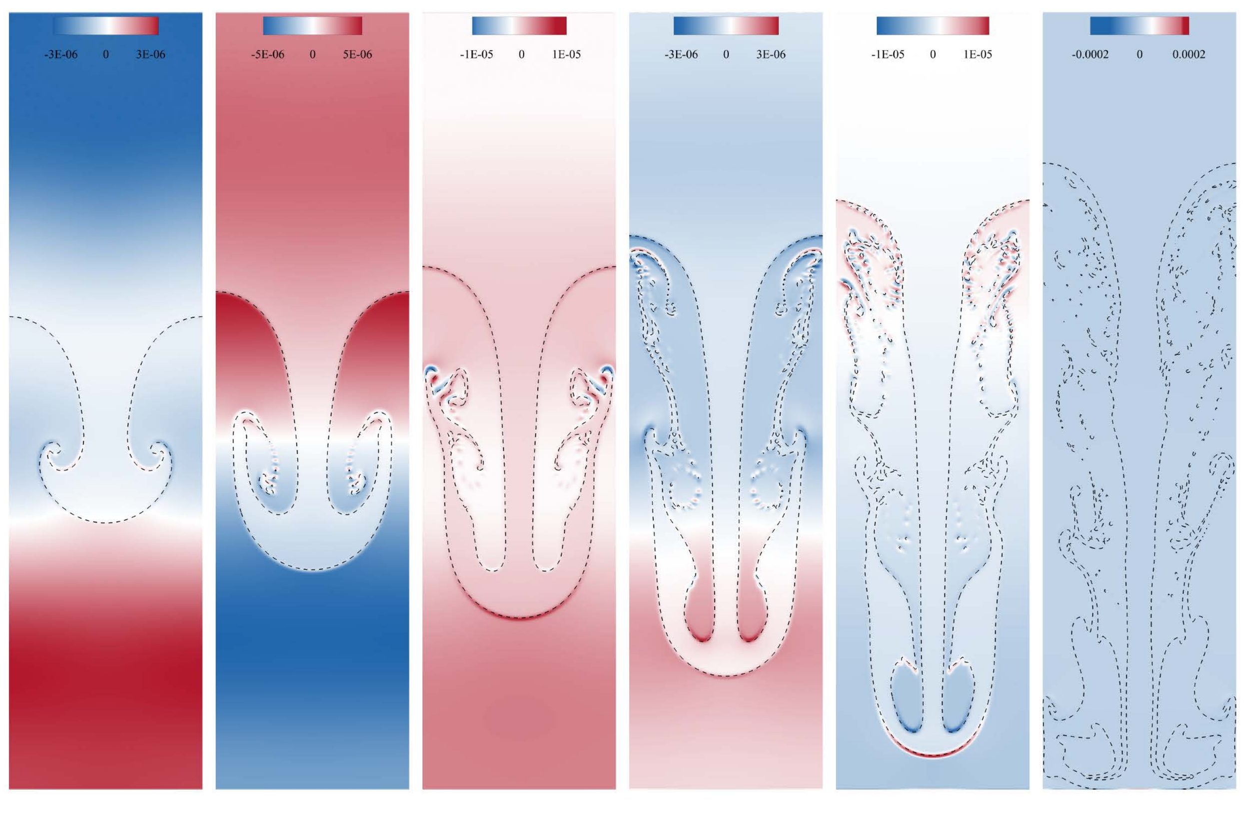
### ❑ Rayleigh-Taylor instability (RTI)

A layer of heavy fluid lies above a lighter fluid in a gravitational field. A strong enough perturbation at the interface results in the replacement of the two fluids. The phase field domain and the divergence of the velocity field ($\boldsymbol{\nabla}.\boldsymbol{u}$) for the one-eq scheme and the two-eq scheme are shown for $\mathrm{Re} = \rho_r\sqrt{gL_0}L_0/\eta_r = 3000$, $\rho^* = \rho_r/\rho_b = 3$, $\eta^* = \eta_r/\eta_b = 1$.



(a) $t^*=1.5$ (b) $t^*=2.0$ (c) $t^*=2.5$ (d) $t^*=3.0$ (e) $t^*=3.5$ (f) $t^*=4.0$

Fig. 1: Phase field of $\phi = 0.5$. The solid black line corresponds to the two-eq scheme, while the solid *red* line indicates the one-eq scheme when the *red* fluid is solved for, and the solid *blue* line indicated the one-eq scheme when the *blue* fluid is solved for.



(a) $t^*=1.5$ (b) $t^*=2.0$ (c) $t^*=2.5$ (d) $t^*=3.0$ (e) $t^*=3.5$ (f) $t^*=4.0$

Fig. 2: Snapshots of the divergence of the velocity field, $\boldsymbol{\nabla}.\boldsymbol{u}$ for the one-eq scheme when the *red* fluid is solved.

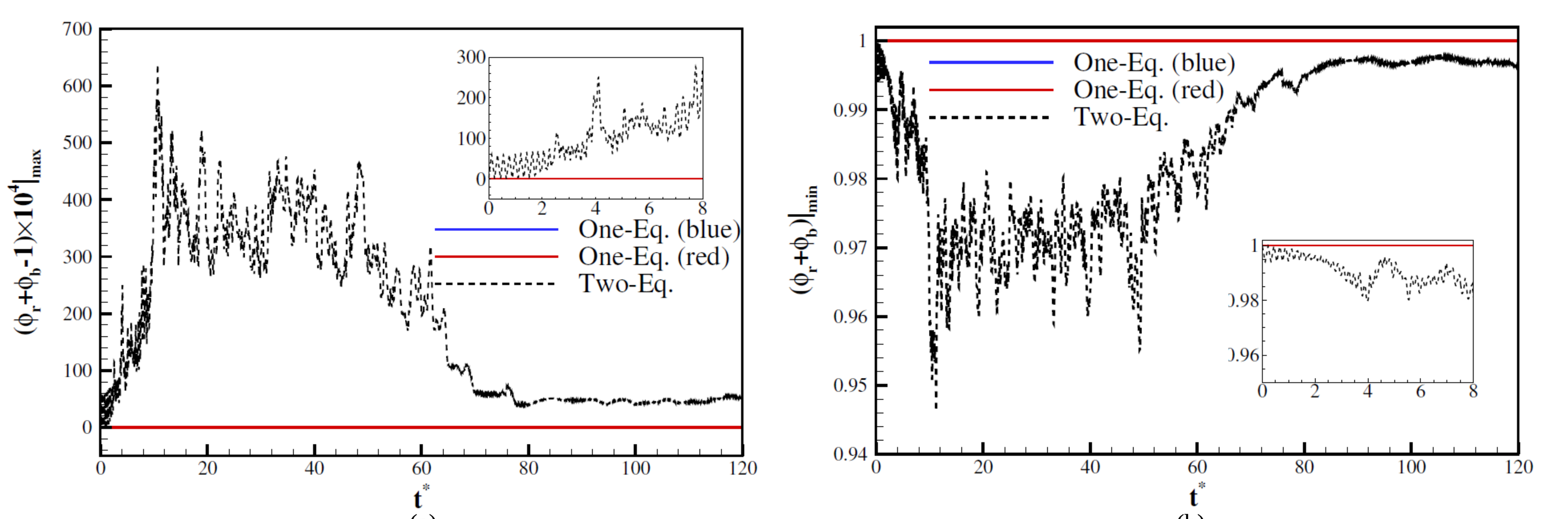


Fig. 3: Temporal evolution of the minimum and maximum of $\phi_r + \phi_b$.

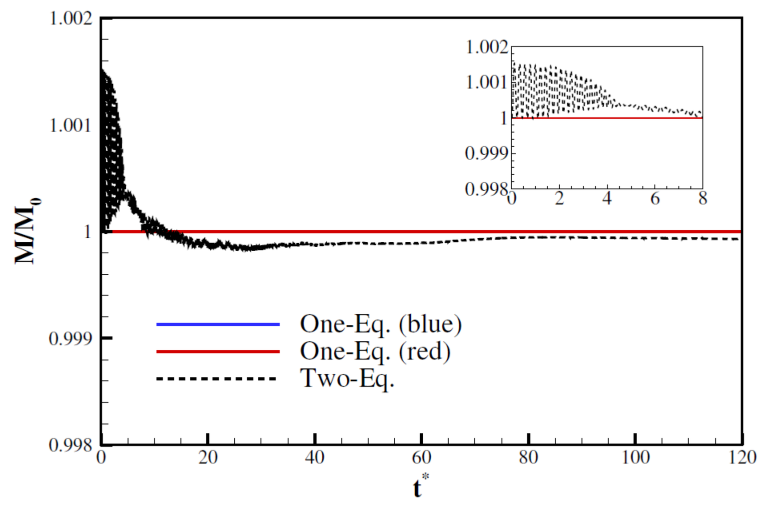


Fig. 4: Temporal evolution of system mass.

Table 1: Computational costs for the RTI benchmark.

| Scheme | Simulation time (second) | Memory (mega byte) |
|---|---|---|
| One-eq scheme | 178298 | 161 |
| Two-eq scheme | 198365 | 202 |

Table 2: Different benchmarks.

| Benchmark | Domain conditions |
|---|---|
| I | $\boldsymbol{\nabla}\cdot\boldsymbol{u} \neq 0$ |
| II | $\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0$ (with singularity) |
| III | $\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0$ (without Singularity) |
| IV | $\boldsymbol{u} = (0,0)$ |

### ❑ Benchmark I

A circular interface is placed at the corner of a square domain with the following shear flow which is reversed at the middle of the simulation:

$$u_x = U_0x/L_0$$
$$u_y = U_0y/L_0$$

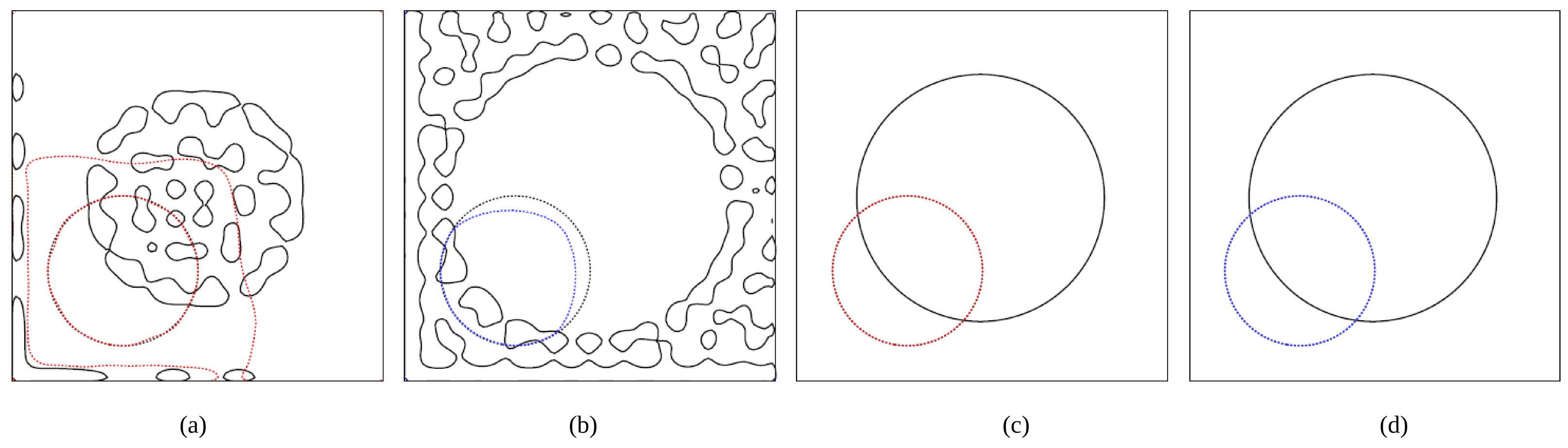


Fig. 5: Benchmark I at Pe=100 and Ch=3/100. One-eq scheme with (a) *red* fluid, (b) *blue* fluid is solved, and two-eq scheme with (c) *red* fluid, (d) *blue* fluid. Initial condition by dashed black, middle time by black solid line, final time by colored lines.

### ❑ Benchmark II

A circular interface is placed at the center of a square domain with the following velocity field with a singularity at the middle of domain which is revered at the middle of the simulation:

$$u_r = U_0/2r$$
$$u_\theta = 0$$

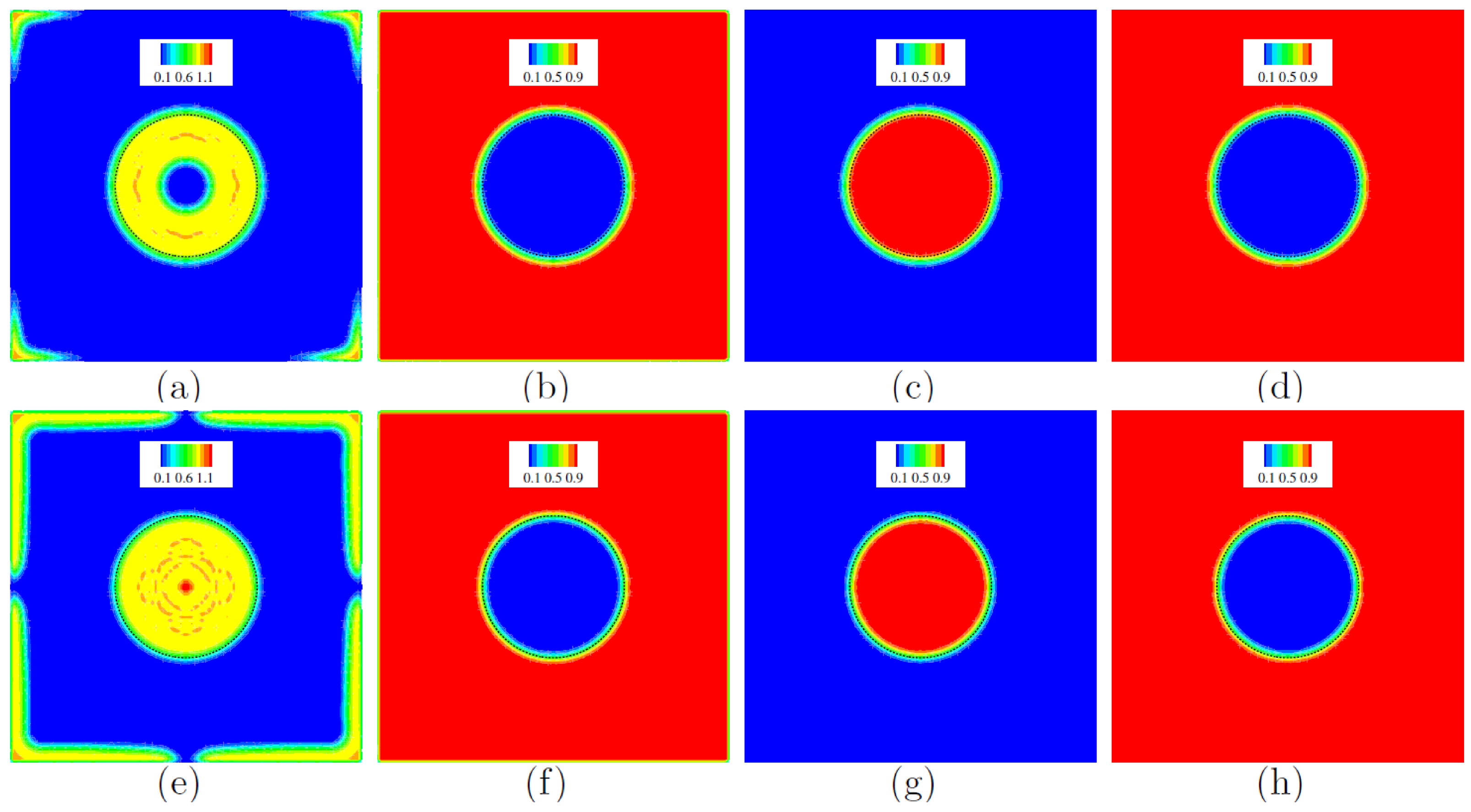


Fig. 6: Benchmark II at Pe=100 and Ch=3/100. One-eq scheme with (a-e) *red* fluid, (b-f) *blue* fluid is solved, and two-eq scheme with (c-g) *red* fluid, (d-h) *blue* fluid.

### ❑ Benchmark III

A circular interface is placed at the bottom of a square domain with the following velocity which is reversed at the middle of the simulation:

$$u_x = U_0\sin^2\left(\frac{\pi x}{L_0}\right)\sin\left(\frac{2\pi y}{L_0}\right)\cos\left(\frac{\pi t}{t_0}\right)$$
$$u_y = -U_0\sin^2\left(\frac{\pi y}{L_0}\right)\sin\left(\frac{2\pi x}{L_0}\right)\cos\left(\frac{\pi t}{t_0}\right)$$

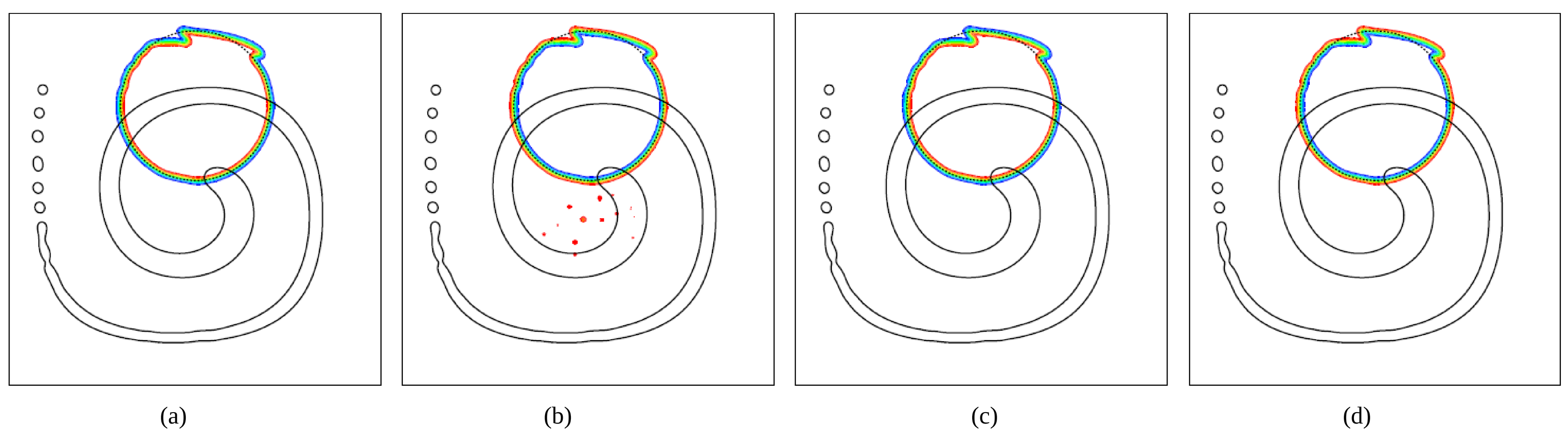


Fig. 7: Benchmark III at Pe=500 and Ch=3/200. One-eq scheme with (a) *red* fluid, (b) *blue* fluid is solved, and two-eq scheme with (c) *red* fluid, (d) *blue* fluid.

### ❑ Benchmark IV

A circular interface is placed at the center of a square domain with the following velocity field:

$$u_x = 0$$
$$u_y = 0$$

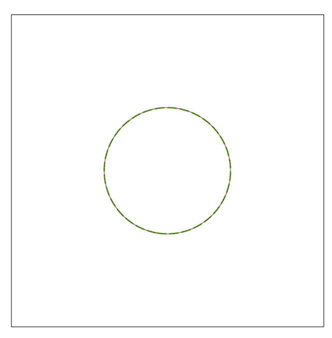


Fig. 8: Benchmark IV.

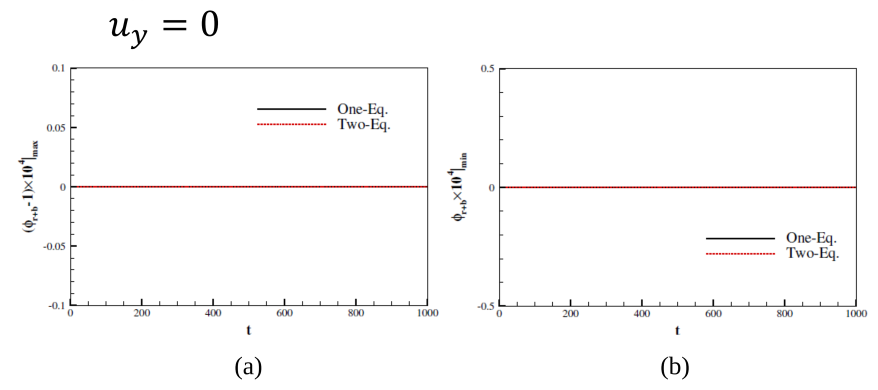


Fig. 9: Temporal evolution of the minimum and maximum of $\phi_r + \phi_b$.

By considering the constraint (1) and solving the interface-capturing equation of the red fluid, the other equation would be:

$$\frac{\partial \phi_b}{\partial t} + \boldsymbol{\nabla}.(\boldsymbol{u}\phi_b) - \boldsymbol{\nabla}.\boldsymbol{u} = D\nabla^2\phi_b + D\frac{4}{\xi}\boldsymbol{\nabla}.\left[\frac{\phi_r\phi_b}{\phi_r+\phi_b}\boldsymbol{n}\right]$$

which includes the extra term $\boldsymbol{\nabla}.\boldsymbol{u}$ which explains the discrepancies between the one-eq and two-eq schemes.

## References

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2- Haghani-Hassan-Abadi, Reza, Mohammad-Hassan Rahimian, and Abbas Fakhari. "Conservative phase-field lattice-Boltzmann model for ternary fluids." Journal of Computational Physics 374 (2018): 668-691.

3- Haghani-Hassan-Abadi, Reza, Abbas Fakhari, and Mohammad-Hassan Rahimian. "Phase-change modeling based on a novel conservative phase-field method." Journal of Computational Physics 432 (2021): 110111.