Efficient solution methods for variable density and variable viscosity Navier-Stokes equations arising in two-phase bubbly flows

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June 19, 2015

Table of contents

Motivation of this work

Mathematical model for bubbly flows

Solution strategy

Numerical experiments

Conclusion

Future work

Motivation of this work

Many applications encounter variable-density and variable-viscosity Navier-Stokes equations, e.g. two phase bubbly flows.

Fast and reliable solution method for the variable-coefficient Navier-Stokes equations is of crucial importance and is the topic of this talk.

Mathematical model for bubbly flows

To simulate the bubbly flows we choose the phase-field models, whose properties consist of

1. the phase-field with distinct values, e.g. -1 and 1, is used to indicate the liquid and gas phases.
2. the interface between the two phases is associated with an intermediate contour of the phase field.
3. the evolution of deformable bubbles and interfaces is described by the evolution of the phase-field.
4. the complex surface-tension induced topological transitions, interactions and moving contact lines of the interfaces are easily and accurately captured.
5. the mass is conserved and the reinitialization is not necessary.

Mathematical model for bubbly flows (Cont.)

The governing equations in the phase-field models include the Cahn-Hilliard and Navier-Stokes equations:

$$CH : \begin{cases} \frac{1}{Pe}\Delta\eta + \frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = 0, \\ \eta - \Psi'(c) + \epsilon^2\Delta c = 0, \end{cases}$$

$$NS : \begin{cases} \rho(c)\frac{\partial(\sqrt{\rho(c)}\mathbf{u})}{\partial t} + (\rho(c)\mathbf{u}\cdot\nabla)\mathbf{u} + \frac{\mathbf{u}}{2}\nabla\cdot(\rho(c)\mathbf{u}) - \frac{1}{Re}\Delta\mathbf{u} + \nabla p = \mathbf{f}, \\ \nabla\cdot\mathbf{u} = 0, \end{cases}$$

- $c \in [-1, 1]$ is the phase-filed; η is the chemical potential and $\Psi(c) = \frac{1}{4}(c^2 - 1)^2$.
- $\rho(c) = \frac{2}{(1-c)/\rho_1 + (1+c)/\rho_2}$, ρ_1, ρ_2 are densities in two phases. (assuming the same viscosity for simplicity)
- Pe, ϵ, Re: the Peclet, interface thickness and Reynolds numbers.
- $\mathbf{f} = \mathbf{f}_{ST} + \mathbf{f}_{BF}$ (ST: surface tension, BF: body force).
  $\mathbf{f}_{ST}$ is a function of (c, η).

Mathematical model for bubbly flows (Cont.)

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$$CH: \begin{cases} \frac{1}{Pe}\Delta\eta + \frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = 0, \\ \eta - \Psi'(c) + \epsilon^2\Delta c = 0, \end{cases}$$

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The coupling and nonlinear terms in the governing equations:

1. coupling terms: $\mathbf{u}\cdot\nabla c$ in CH; $\rho(c)$ and $\mathbf{f}_{ST}(c,\eta)$ in NS
2. nonlinear terms: $\Psi(c) = \frac{1}{4}(c^2-1)^2$ in CH; $(\rho(c)\mathbf{u}\cdot\nabla)\mathbf{u}$ and $\frac{\mathbf{u}}{2}\nabla\cdot(\rho(c)\mathbf{u})$ in NS

Solution strategy

$$CH: \begin{cases} \frac{1}{Pe}\Delta\eta + \frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = 0, \\ \eta - \Psi'(c) + \epsilon^2\Delta c = 0, \end{cases}$$

$$NS: \begin{cases} \rho(c)\frac{\partial(\sqrt{\rho(c)}\mathbf{u})}{\partial t} + (\rho(c)\mathbf{u}\cdot\nabla)\mathbf{u} + \frac{\mathbf{u}}{2}\nabla\cdot(\rho(c)\mathbf{u}) - \frac{1}{Re}\Delta\mathbf{u} + \nabla p = \mathbf{f}, \\ \nabla\cdot\mathbf{u} = 0, \end{cases}$$

Use the explicit splitting time integration method at the time level $n+1$:

Step 1: substitute $\mathbf{u}^n$ into the CH equation and compute (c^{n+1}, η^{n+1}) simultaneously by Newton-Krylov method.

Step 2: recover ρ^{n+1} as $\rho^{n+1} = \frac{2}{(1-c^{n+1})/\rho_1 + (1+c^{n+1})/\rho_2}$

Step 3: substitute ρ^{n+1} into the NS equation and compute $(\mathbf{u}^{n+1}, p^{n+1})$ simultaneously by Newton-Krylov method.

Step 4: proceed to the next time level $n+2$.

Solution strategy (Cont.)

Step 1: compute (c^{n+1}, η^{n+1}) simultaneously by solving

$$\eta^{n+1} - \Psi'(c^{n+1}) + \epsilon^2 \Delta c^{n+1} = 0,$$
$$-\frac{1}{Pe}\Delta\eta^{n+1} + \frac{\partial c^{n+1}}{\partial t} + (\mathbf{u}^n \cdot \nabla) c^{n+1} = 0,$$

Step 2: Recover ρ^{n+1} as $\rho^{n+1} = \frac{2}{(1-c^{n+1})/\rho_1 + (1+c^{n+1})/\rho_2}$

Step 3: compute $(\mathbf{u}^{n+1}, p^{n+1})$ simultaneously by solving

$$\begin{aligned}\sqrt{\rho^{n+1}}\frac{\partial(\sqrt{\rho^{n+1}}\mathbf{u}^{n+1})}{\partial t} + (\rho^{n+1}\mathbf{u}^{n+1}\cdot\nabla)\mathbf{u}^{n+1} + \frac{\mathbf{u}^{n+1}}{2}\nabla\cdot(\rho^{n+1}\mathbf{u}^{n+1}) & \\ -\nu\Delta\mathbf{u}^{n+1} + \nabla p^{n+1} &= \mathbf{f}^{n+1}, \\ \nabla\cdot\mathbf{u}^{n+1} &= 0.\end{aligned}$$

Solution strategy (Cont.)

Substitute first-order backward Euler and second-order BDF stepping methods, i.e.,

$$\frac{\partial c^{n+1}}{\partial t} = \frac{c^{n+1} - c^{n}}{\Delta t}, \quad \frac{3c^{n+1} - 4c^{n} + c^{n-1}}{2\Delta t}$$

$$\frac{\partial(\sqrt{\rho^{n+1}}\mathbf{u}^{n+1})}{\partial t} = \frac{\sqrt{\rho^{n+1}}\mathbf{u}^{n+1} - \sqrt{\rho^{n}}\mathbf{u}^{n}}{\Delta t}, \quad \frac{3\sqrt{\rho^{n+1}}\mathbf{u}^{n+1} - 4\sqrt{\rho^{n}}\mathbf{u}^{n} + \sqrt{\rho^{n-1}}\mathbf{u}^{n-1}}{2\Delta t}$$

At any time level N, i.e. $t = N\Delta t$, we have the results:

- $\| (\sqrt{\rho}\mathbf{u})^N \|_{L^2} \leq \| \sqrt{\rho_0}\mathbf{u}_0 \|_{L^2}$
- $\int_\Omega \nabla \cdot \mathbf{u}^N = 0$

Solution strategy (Cont.)

At each time level, Newton-Krylov method is used to solve the nonlinear Navier-Stokes equations. At each Newton iteration, the linearised system after the spacial discretization is of the block two-by-two structure:

$$\begin{bmatrix} A & B^T \\ B & O \end{bmatrix} \begin{bmatrix} \mathbf{u}_h \\ p_h \end{bmatrix} = \begin{bmatrix} R_u \\ R_p \end{bmatrix}, \quad \text{or} \quad \mathcal{A}\mathbf{x} = \mathbf{b}.$$

The preconditioner is of the block lower-triangular form

$$\mathcal{P} = \begin{bmatrix} A & O \\ B & -\widetilde{S} \end{bmatrix},$$

- $S_{\mathcal{A}} = BA^{-1}B^T \approx B(O(\tau^{-1})M)^{-1}B^T \approx O(\tau)B\widetilde{M}^{-1}B^T = \widetilde{S}$ ($\widetilde{M}$ is the diagonal of velocity mass matrix),
- algebraic multigrid solutions methods with proper stopping tolerance are used for subsystems with A and $\widetilde{S}$.

Numerical experiments

We compute the evolution of a Rayleigh-Taylor instability in the rectangular domain$[0, 1] \cup [0, 4]$, consisting of two immiscible liquids.

At $t = 0$ the heavier liquid is located above the lighter, and for $t > 0$, the system is driven by the gravity force.

Numerical experiments - preliminary

- Finite element method is used for the space discretization. Q_2 basis function is used for the velocity, concentration and chemical potential. Q_1 basis function is used for pressure.
- Second-order BDF scheme is used for the time discretization.
- Relative stopping tolerance for Newton iterations is 10^{-8}. GCR method is chosen to solve the linear system at each Newton iteration, and its relative stopping tolerance is 10^{-2}.
- To solve velocity and pressure subsystems at each GCR iteration, we use an aggregation-based multigrid solver `agmg`, and its relative stopping tolerance is 10^{-2}.

Numerical experiments - efficiency

Table: Implicit scheme: the number of iterations at one time level. $h = 1/2^6$.

ρ_2/ρ_1	3	7	15	30	50	100
			$Re = 1000$			
nonlinear iter.	4	4	4	4	4	4
linear iter.	3	4	5	5	6	8
agmg iter. for $\mathbf{u}$	2	2	3	3	3	3
agmg iter. for p	3	3	3	3	3	3
			$Re = 5000$			
nonlinear iter.	4	4	4	4	4	4
linear iter.	4	4	5	5	6	8
agmg iter. for $\mathbf{u}$	2	2	3	3	3	3
agmg iter. for p	3	3	3	3	3	3

The solution method is independent of the density ratio and Reynolds number.

Numerical experiments - efficiency (Cont.)

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Table: Implicit scheme: the number of iterations at each time level.
$Re = 5000$, $\rho_2/\rho_1 = 7$.

mesh size	$h = 1/2^4$	$h = 1/2^5$	$h = 1/2^6$	$h = 1/2^7$
nonlinear iter.	4	4	4	4
linear iter.	4	4	4	4
agmg iter. for $\mathbf{u}$	2	2	2	2
agmg iter. for p	3	3	3	3

The solution method is independent of the mesh size.

Numerical experiments - plots

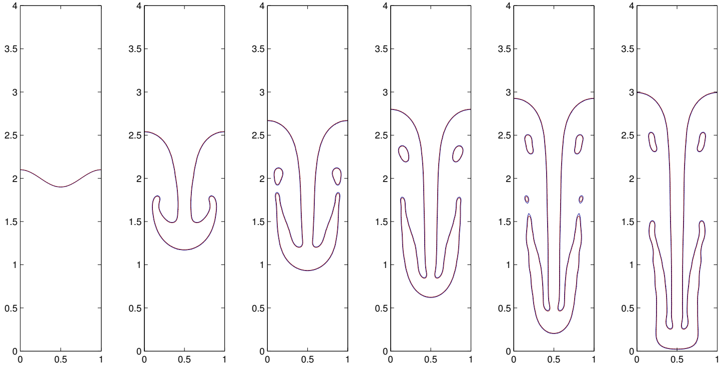

Figure: the interface for $Re = 1000$, $\rho_2/\rho_1 = 3$ and $h = 1/2^6$, $t = 0, 2.0, 2.5, 3.0, 3.5, 3.75$.

Numerical experiments - plots (Cont.)

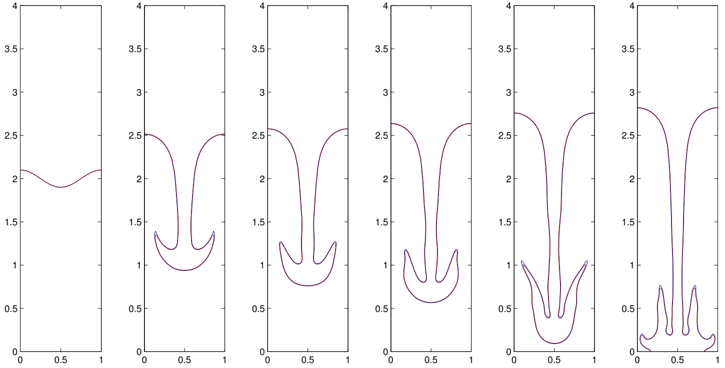

Figure: the interface for $Re = 1000$, $\rho_2/\rho_1 = 7$ and $h = 1/2^6$, $t = 0, 2.0, 2.25, 2.5, 3.0, 3.25$.

Conclusion

The proposed Newton-Krylov solution method and the preconditioner for the variable-coefficient Navier-Stokes equations are quite efficient and robust with respect to density ratio, mesh size and Reynolds number.

Future work

The drawbacks of the explicit splitting time integration scheme:

1. a severe restriction on the time-step size is needed for stability reasons. The maximum time-step size is many orders of magnitude smaller than the time span of evolutional phenomena.
2. limited temporal accuracy, at most second order.

Planned alternative: fully coupled Navier-Stokes-Cahn-Hilliard + diagonally implicit Runge-Kutta integrators. The advantages:

1. unconditionally stable for any time-step sizes;
2. arbitrary high-order temporal accuracy;
3. desired accuracy can be achieved with large time-step sizes.

Future work

For the fully coupled and nonlinear Navier-Stokes-Cahn-Hilliard equation at each stage of the Runge-Kutta schemes, the linearised system arising in Newton method is of the following form:

$$\begin{bmatrix} A_{NS} & C_1 \\ C_2 & A_{CH} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{NS} \\ \mathbf{x}_{CH} \end{bmatrix} = \begin{bmatrix} R_{NS} \\ R_{CH} \end{bmatrix},$$

where A_{NS} and A_{CH} are the matrices arising in the Navier-Stokes and Cahn-Hilliard equations and C_1 and C_2 denote the coupling terms.

The open question is how to precondition the above two-by-two system. One possible preconditioner is

$$\begin{bmatrix} P_{NS} & O \\ C_2 & P_{CH} \end{bmatrix} (S = A_{CH} - C_2 A_{NS}^{-1} C_1)$$

where known preconditioners for the individual systems can be applied.

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