Part IV: Numerical schemes for the phase-filed model

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The complete set of governing equations

Find $u,\ p,\ (\phi,\xi)$ such that

$$\rho(u_t+(u\cdot\nabla)u)+\nabla p=\nabla\cdot\mu(\nabla u+\nabla^t u)-\lambda\nabla\cdot(\nabla\phi\otimes\nabla\phi);$$
$$\nabla\cdot u=0;$$
$$\phi_t+(u\cdot\nabla)\phi=\gamma(\Delta\phi-f(\phi)+\xi(t)),$$
$$\frac{d}{dt}\int_\Omega\phi dx=0;$$
$$(\rho,\mu)=\frac{1+\phi}{2}(\rho_1,\mu_1)+\frac{1-\phi}{2}(\rho_2,\mu_2).$$

Remark: No energy law for this system.

Time discretization of the full system

$$\rho^n \frac{u^{n+1} - u^n}{\delta t} - \nabla \cdot \mu^n D(u^{n+1}) + \nabla p^n = \text{expl. nonl. terms;}$$

$$(\frac{1}{\rho^n} \nabla \psi^{n+1}, \nabla q) = (\frac{u^{n+1} - u^n}{\delta t}, \nabla q),$$

$$p^{n+1} = \psi^{n+1} + p^n + \nu \nabla \cdot u^{n+1};$$

$$\frac{\phi^{n+1} - \phi^n}{\delta t} - \gamma(\Delta - \frac{C_s}{\eta^2} I)\phi^{n+1} = \gamma \xi^{k+1} + \text{expl. nonl. terms,}$$

$$\int_\Omega \phi^{k+1} dx = \int_\Omega \phi^k dx;$$

$$(\rho^{n+1}, \mu^{n+1}) = \frac{1 + \phi^{n+1}}{2}(\rho_1, \mu_1) + \frac{1 - \phi^{n+1}}{2}(\rho_2, \mu_2).$$

Summary:

- Only a sequence of **elliptic equations** needs to be solved at each time step:

- The variable-coefficient term

$$-\nabla \cdot (\mu^n \nabla u^{n+1})$$

can be approximated by

$$-\bar{\mu}\Delta u^{n+1} - \nabla \cdot (\mu^n - \bar{\mu})\nabla u^n,$$

where $\bar{\mu}$ is some average of $\mu(\phi)$;

• the same trick can not be applied to

$$(\frac{1}{\rho^n}\nabla\psi^{n+1}, \nabla q) = (\frac{u^{n+1} - u^n}{\delta t}, \nabla q).$$

• For problems with relatively small density ratio, one can use the so called Boussinesq approximation: replacing ρ by a constant and accounting the density difference through a gravity force.

• Volume of ϕ is conserved for all time.

• Only limited stability and error analysis were available for the constant density case.

- Second-order accurate schemes can be constructed easily.

- The above scheme is very easy to implement as the main building blocks are elliptic/fast Poisson solvers. However, two challenges remains:

  - The elliptic solve for the pressure becomes very expensive as the density ratio becomes large.

  - The time step is mainly constraintly by the explict treatment of the surface tension term.

The new formulation with energy law

Let $\sigma = \sqrt{\rho}$. Find $u,\ p,\ (\phi, \xi)$ such that

$$
\begin{aligned}
&\sigma(\sigma u)_t + (\rho u \cdot \nabla)u + \frac{1}{2}\nabla \cdot (\rho u)u + \nabla p \\
&\qquad\qquad = \nabla \cdot \mu(\nabla u + \nabla^t u) - \lambda \nabla \cdot (\nabla \phi \otimes \nabla \phi); \\
&\nabla \cdot u = 0; \\
&\phi_t + (u \cdot \nabla)\phi = \gamma(\Delta \phi - f(\phi) + \xi(t)), \\
&\frac{d}{dt}\int_\Omega \phi dx = 0; \\
&(\rho, \mu) = \frac{1+\phi}{2}(\rho_1, \mu_1) + \frac{1-\phi}{2}(\rho_2, \mu_2).
\end{aligned}
$$

The gauge-Uzawa scheme for the new model

$$\sigma^{n+1}\frac{\sigma^{n+1}\tilde{u}^{n+1}-\sigma^n u^n}{\delta t}+\rho^n(u^n\cdot\nabla)\tilde{u}^{n+1}+\frac{1}{2}(\nabla\cdot(\rho^n u^n))\tilde{u}^{n+1}$$
$$-\mu\Delta\tilde{u}^{n+1}+\mu\nabla s^n+\lambda\Delta\rho^{n+1}\nabla\rho^{n+1}=0,$$
$$\tilde{u}^{n+1}|_{\partial\Omega}=0;$$

$$-\nabla\cdot(\frac{1}{\rho^{n+1}}\nabla\psi^{n+1})=\nabla\cdot\tilde{u}^{n+1},\quad \partial_n\psi^{n+1}=0;$$
$$u^{n+1}=\tilde{u}^{n+1}+\frac{1}{\rho^{n+1}}\nabla\psi^{n+1},$$
$$s^{n+1}=s^n-\nabla\cdot\tilde{u}^{n+1};$$

$$\frac{\rho^{n+1}-\rho^n}{\delta t}+(\tilde{u}^{n+1}\cdot\nabla)\rho^{n+1}-\gamma(\Delta\rho^{n+1}-g(\rho^{n+1}))=0,$$
$$\partial_n\rho^{n+1}|_{\partial\Omega}=0.$$

- Thanks to the energy law for the density based phase-field model, we are able to prove that the above scheme is unconditionally stable. In practice, we treat the nonlinear terms explicitly.
- Second-order version can be constructed.
- Still need to solve a pressure equation with variable coefficients.

To avoid solving a pressure equation with variable coefficients, we consider a pressure-stabilized formulation of NSE (Rannacher '92, S. '93):

$$\rho^\epsilon(u_t^\epsilon + (u^\epsilon \cdot \nabla)u^\epsilon) = \mu\Delta u^\epsilon - \nabla p^\epsilon + \rho^\epsilon f,$$
$$\rho_t^\epsilon + (u^\epsilon \cdot \nabla)\rho^\epsilon = 0,$$

with

$$\nabla \cdot u^\epsilon - \epsilon\Delta p^\epsilon = 0, \quad \frac{\partial p^\epsilon}{\partial n}|_{\partial\Omega} = 0,$$

or

$$\nabla \cdot u^\epsilon - \epsilon\Delta p_t^\epsilon = 0, \quad \frac{\partial p_t^\epsilon}{\partial n}|_{\partial\Omega} = 0.$$

Notice that only a pressure Poisson equation is involved.

A new scheme for the density based phase-field model:

$$\sigma^{n+1}\frac{\sigma^{n+1}u^{n+1}-\sigma^n u^n}{\delta t}+\rho^n(u^n\cdot\nabla)u^{n+1}$$
$$-\nabla\cdot\mu^n\nabla u^{n+1}+\nabla p^n+\lambda\Delta\rho^{n+1}\nabla\rho^{n+1}=0,$$
$$u^{n+1}|_{\partial\Omega}=0;$$

$$\Delta p^{n+1}=\frac{\rho_{min}}{\delta t}\nabla\cdot u^{n+1},\qquad \partial_n p^{n+1}|_{\partial\Omega}=0;$$

$$\frac{\rho^{n+1}-\rho^n}{\delta t}+(u^{n+1}\cdot\nabla)\rho^{n+1}-\gamma(\Delta\rho^{n+1}-g(\rho^{n+1}))=0,$$
$$\partial_n\rho^{n+1}|_{\partial\Omega}=0.$$

An improved scheme based on pressure-correction:

$$\frac{\rho^{n+1}u^{n+1}-\rho^n u^n}{\delta t}+\rho^n(u^n\cdot\nabla)u^{n+1}+\frac{1}{2}(\nabla\cdot(\rho^n u^n))u^{n+1}$$
$$-\nabla\cdot\mu^n\nabla u^{n+1}+\nabla(p^n+\psi^n)+\lambda\Delta\rho^{n+1}\nabla\rho^{n+1}=0,$$
$$u^{n+1}|_{\partial\Omega}=0;$$

$$\Delta\psi^{n+1}=\frac{\chi}{\delta t}\nabla\cdot u^{n+1},\quad \partial_n\psi^{n+1}|_{\partial\Omega}=0,$$
$$p^{n+1}=p^n+\psi^{n+1};$$

$$\frac{\rho^{n+1}-\rho^n}{\delta t}+(u^{n+1}\cdot\nabla)\rho^{n+1}-\gamma(\Delta\rho^{n+1}-g(\rho^{n+1}))=0,$$
$$\partial_n\rho^{n+1}|_{\partial\Omega}=0.$$

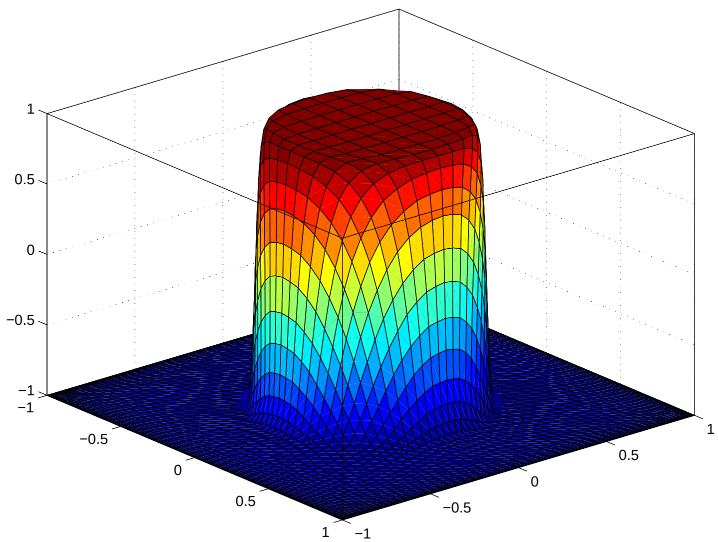
Several remarks:

- Second-order schemes based on pressure-correction can be constructed.
- For problems with large density ratios, the schemes based on pressure-correction are as accurate and much more efficient, when compared with the gauge-Uzawa method.

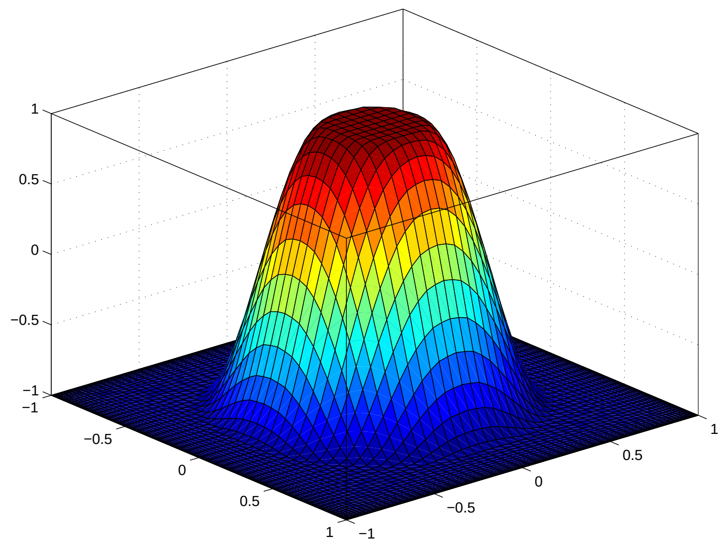
Moving mesh method — r-refinement

Goal: redistribute points, through a smooth mapping, to resolve thin interfaces/regions with large gradients.

Approach: Given a function $u(x;t)$, it amounts to find a suitable "smooth" mapping $\xi = \xi(x;t)$ such that $v(\xi;t) := u(x(\xi;t),t)$ is well-behaved.



$u(x)$ in Ω_P



$u(x)$ in Ω_C

An effective way to find such a mapping is to

$$\min_{x(\xi;t)} \int_{\Omega_c} \sqrt{1+\beta^2 v_\xi^2}\, d\xi$$

which can be approximated by solving a nonlinear moving mesh PDE (Huang '01, Ren & Wang '00, Ceniceros & Hou '01, Du et al. '06):

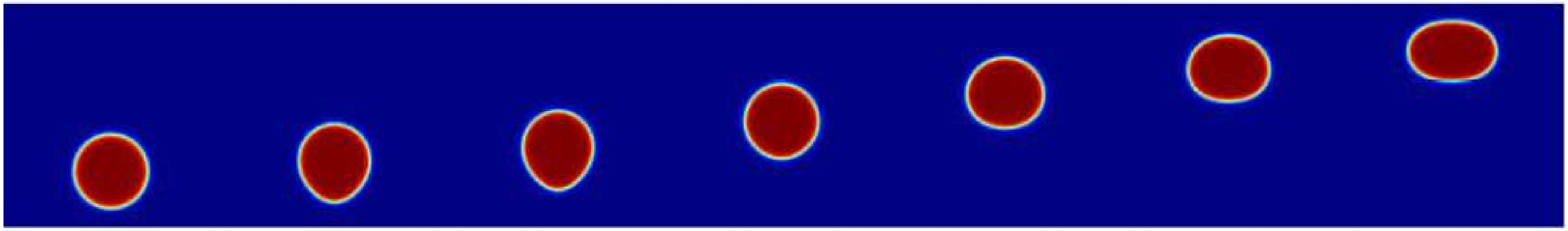
$$\frac{\partial x}{\partial t} = \tau \sum_{i,j=1}^{d} (a^i \cdot a^j) \frac{\partial}{\partial \xi^i}\left(\sqrt{1+\beta^2 |\nabla_\xi v|^2} \frac{\partial x}{\partial \xi^j}\right)$$

with $a^i = \nabla_x \xi^i$.

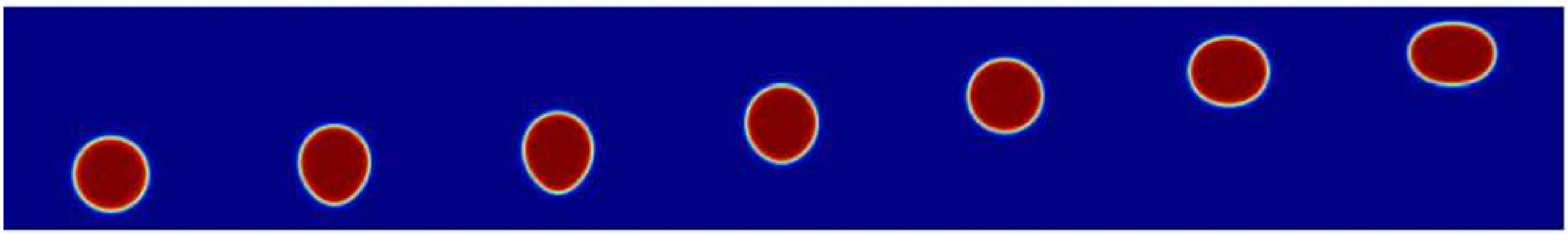
- With the coordinate transform, the elliptic operator with constant coefficients will become one with variable coefficients, but can still be solved using a suitable problem with constant coefficients as preconditioner.

- Typically a moving mesh strategy can reduce the number of points needed in each direction by a factor of 3-4, leading to significantly savings, particularly in 3-D.

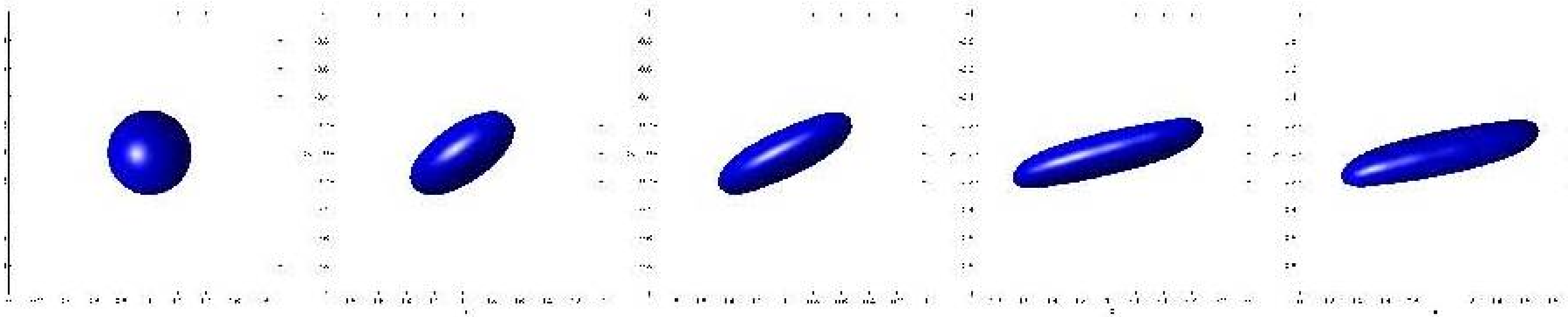
- We are currently developing an adaptive (Legendre polynomial based) multi-wavelet method which is capable to further reduce the total number of points.



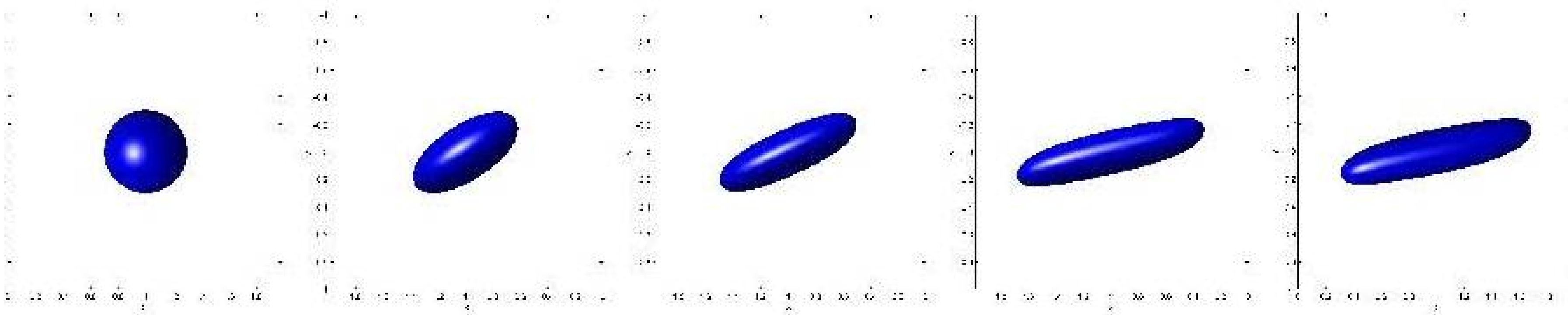
(a) MMM with a grid size of 75^2



(b) FGM with a grid size of 257^2



(a) MMM with a grid size of 33^3



(b) FGM with a grid size of 129^3

Two-phase Newtonian flow with large density ratios: air bubble in water

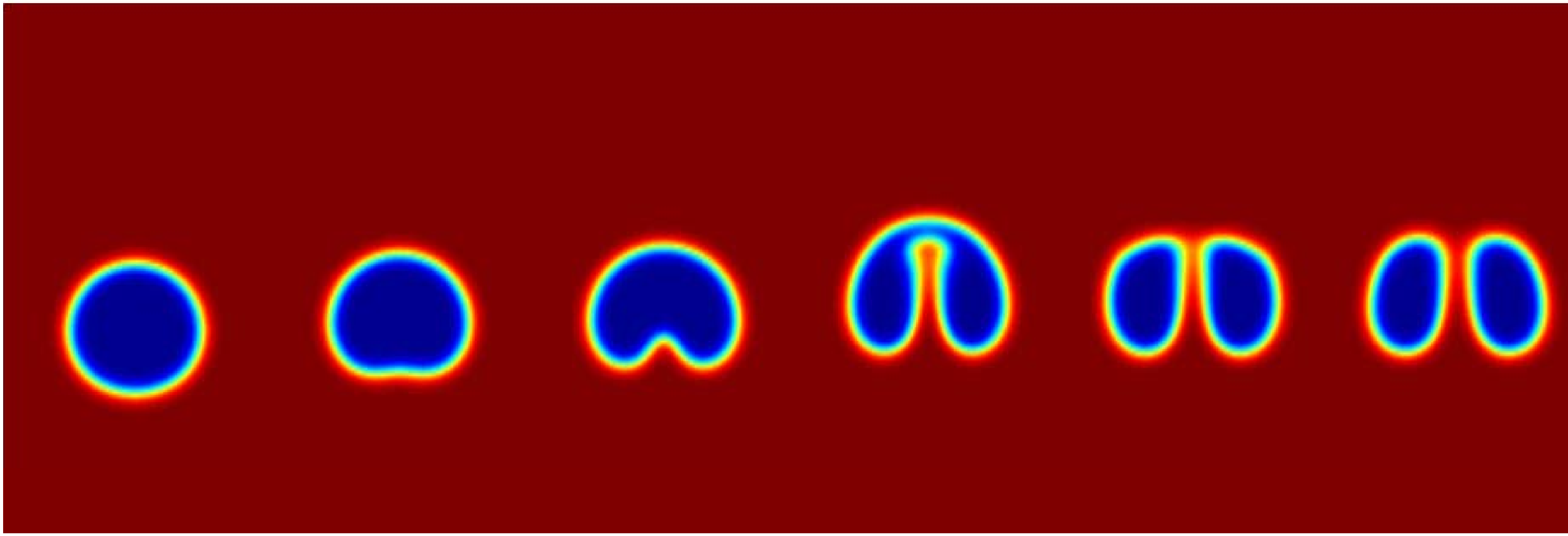
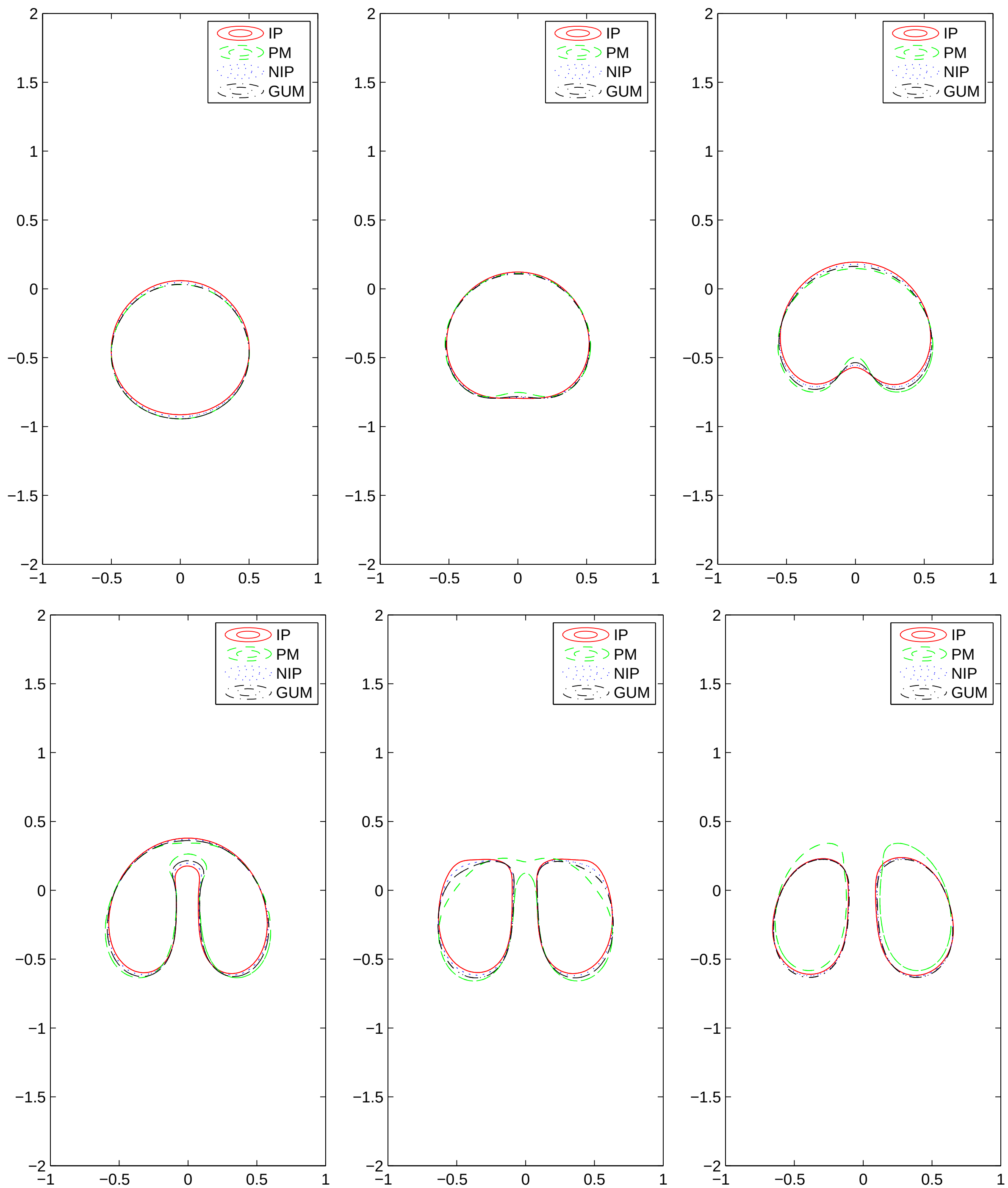


Figure 1: $\rho_1 = 1.16$ and $\rho_{max} = 995$ and homogenous viscosity $\mu = 0.0000186$ at $t = 0.5, 0.75, 1, 1.5, 1.75, 2$.


IP
PM
NIP
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2
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−1.5
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0
0.5
1

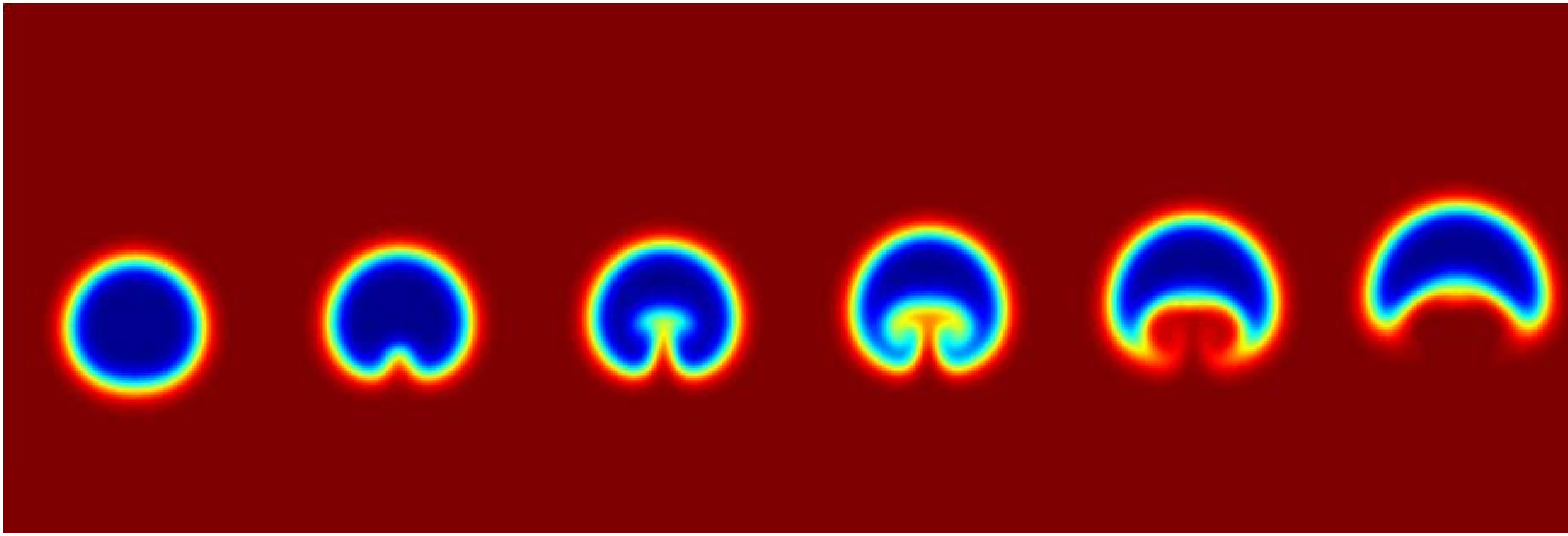
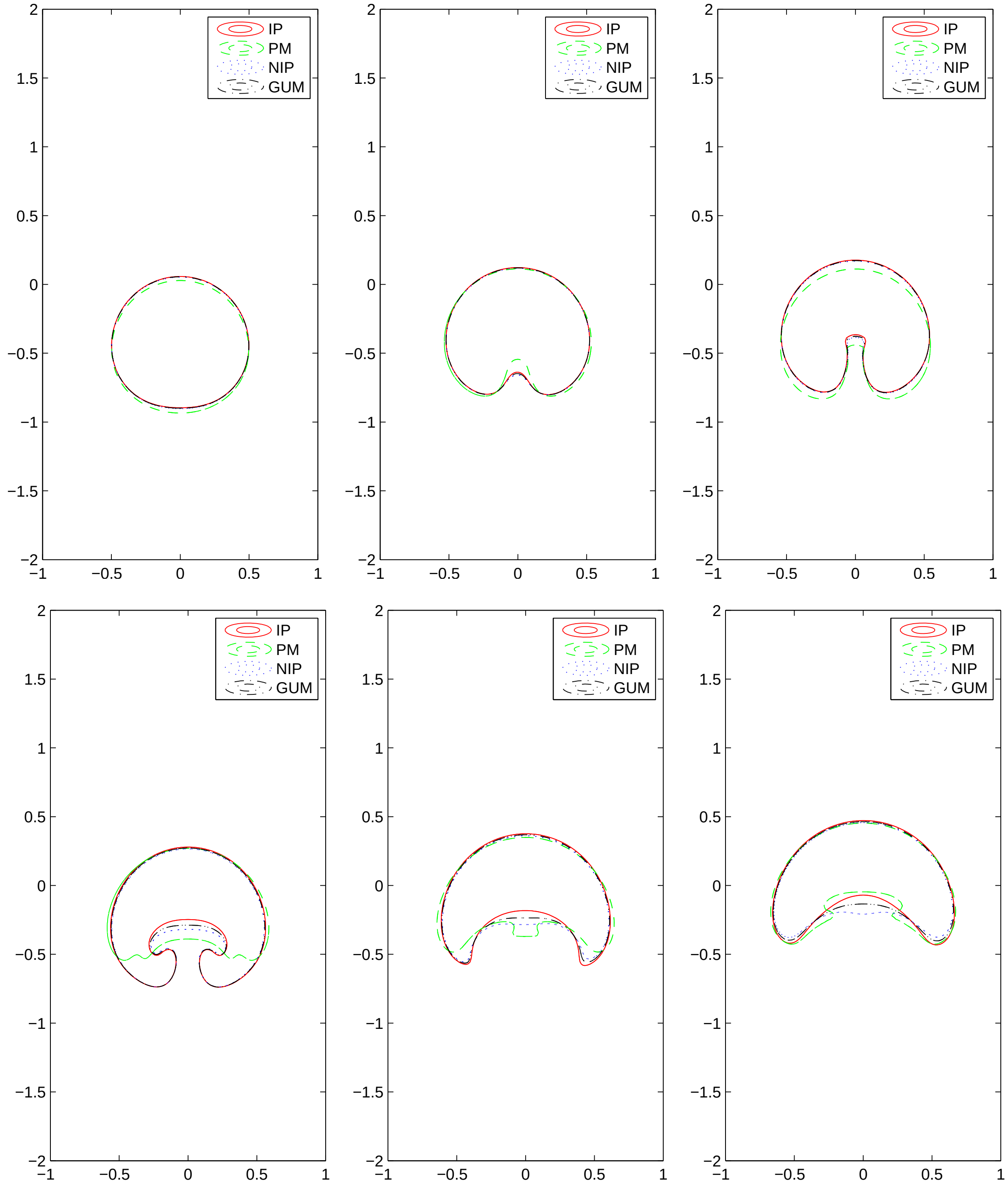


Figure 3: $\rho_1 = 1.16$, $\mu_1 = 0.0000186$ and $\rho_2 = 995$, $\mu_2 = 0.0007977$ at $t = 0.5, 0.75, 1, 1.5, 1.75, 2$.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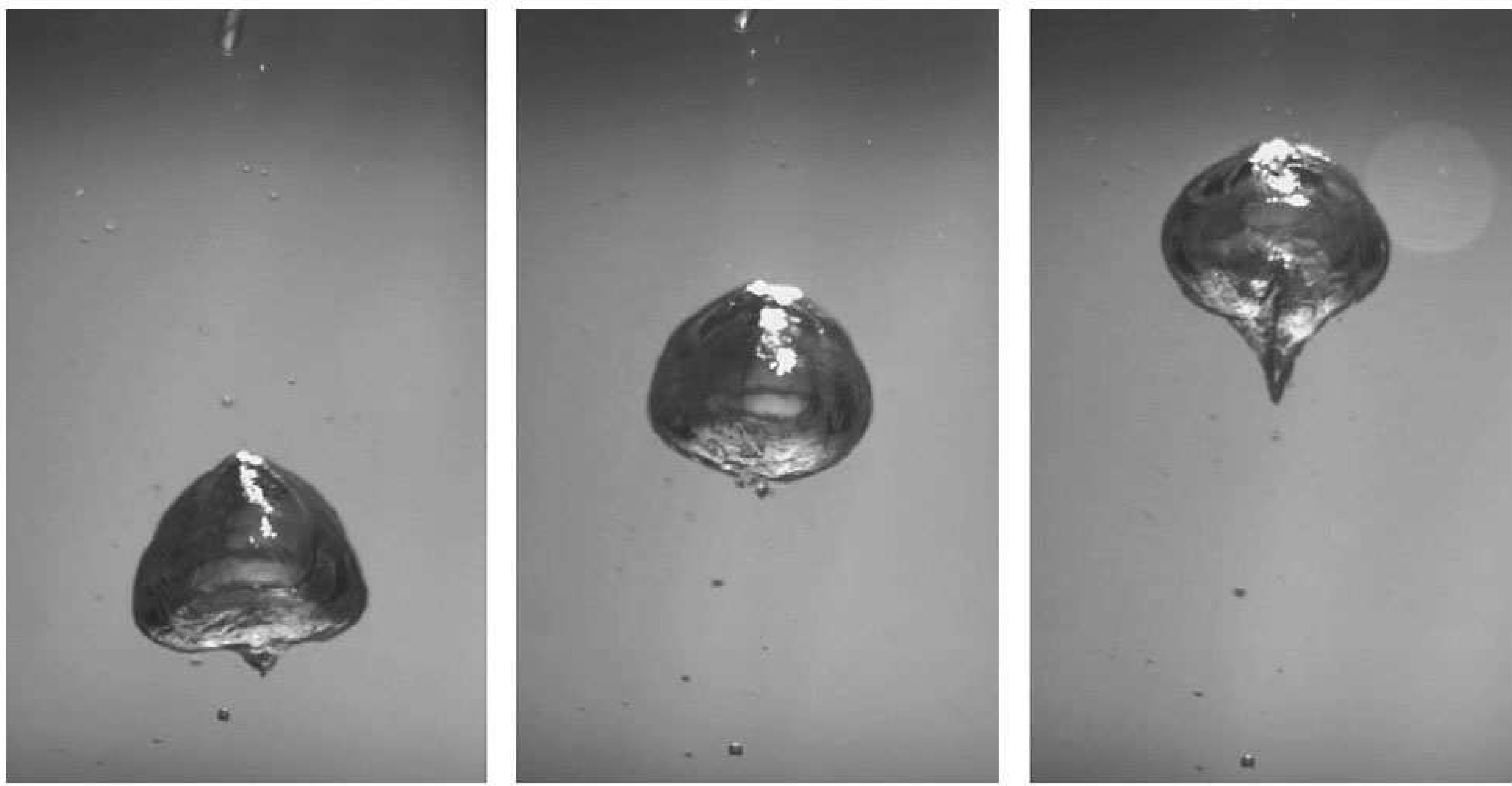


Figure 5: inverted heart shape in experiment by Akers & Belmonte '06: air bubble rising in a polymeric fluid

Mixture of nematic liquid crystals and a Newtonian fluid

Let $\phi = -1$ representing the liquid crystal drop (represented by director $\boldsymbol{n}$) and $\phi = 1$ representing the Newtonian fluid.

Mixing energy density:

$$f_{mix}(\phi, \nabla\phi) = \frac{\lambda}{2}|\nabla\phi|^2 + \frac{\lambda}{4\eta^2}(\phi^2 - 1)^2,$$

Bulk energy density:

$$f_{bulk} = K\left[\frac{1}{2}\nabla\boldsymbol{n} : (\nabla\boldsymbol{n})^{\mathrm{T}} + \frac{(|\boldsymbol{n}|^2 - 1)^2}{4\delta^2}\right],$$

Anchoring energy density:

$$f_{anch} = \frac{A}{2}(\boldsymbol{n} \cdot \nabla\phi)^2,$$

Total energy:

$$F(\phi, \boldsymbol{n}, \nabla\phi, \nabla\boldsymbol{n}) = \int_\Omega f_{mix} + \frac{1+\phi}{2} f_{bulk} + f_{anch}$$

where $(1+\phi)/2$ is the volume fraction of the nematic component.

Governing equations

$$\frac{\partial \phi}{\partial t} + \boldsymbol{v} \cdot \nabla \phi = \gamma_1 \nabla^2 \frac{\delta F}{\delta \phi} \quad \text{(Cahn-Hilliard)} \quad \text{or,}$$

$$\frac{\partial \phi}{\partial t} + \boldsymbol{v} \cdot \nabla \phi = -\gamma_1 \frac{\delta F}{\delta \phi} \quad \text{(Allen-Cahn) + a Lagrange multiplier,}$$

$$\frac{\partial \boldsymbol{n}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{n} = -\gamma_2 \frac{\delta F}{\delta \boldsymbol{n}},$$

$$\nabla \cdot \boldsymbol{v} = 0,$$

$$\rho_0 \left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} \right) = -\nabla p + \nabla \cdot \left[\mu (\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T) + \boldsymbol{\tau}^{\boldsymbol{e}} \right] + g(\rho),$$

where γ_1 is the interfacial mobility and γ_2 determines the relaxation time of $\boldsymbol{n}$, with

$$\frac{\delta F}{\delta \phi} = \lambda \left[-\nabla^2 \phi + \frac{\phi(\phi^2 - 1)}{\eta^2} \right] + \frac{1}{2} f_{bulk} - A \nabla \cdot \left[(\boldsymbol{n} \cdot \nabla \phi) \boldsymbol{n} \right],$$

$$\frac{\delta F}{\delta \boldsymbol{n}} = -K \left[-\nabla \cdot \left(\frac{1+\phi}{2} \nabla \boldsymbol{n} \right) + \frac{1+\phi}{2} \frac{(\boldsymbol{n}^2 - 1)\boldsymbol{n}}{\delta^2} \right] - A(\boldsymbol{n} \cdot \nabla \phi) \nabla \phi,$$

$$\boldsymbol{\tau}^e = -\lambda (\nabla \phi \otimes \nabla \phi) - K \frac{1+\phi}{2} (\nabla \boldsymbol{n}) \cdot (\nabla \boldsymbol{n})^{\mathrm{T}} - A(\boldsymbol{n} \cdot \nabla \phi) \boldsymbol{n} \otimes \nabla \phi.$$

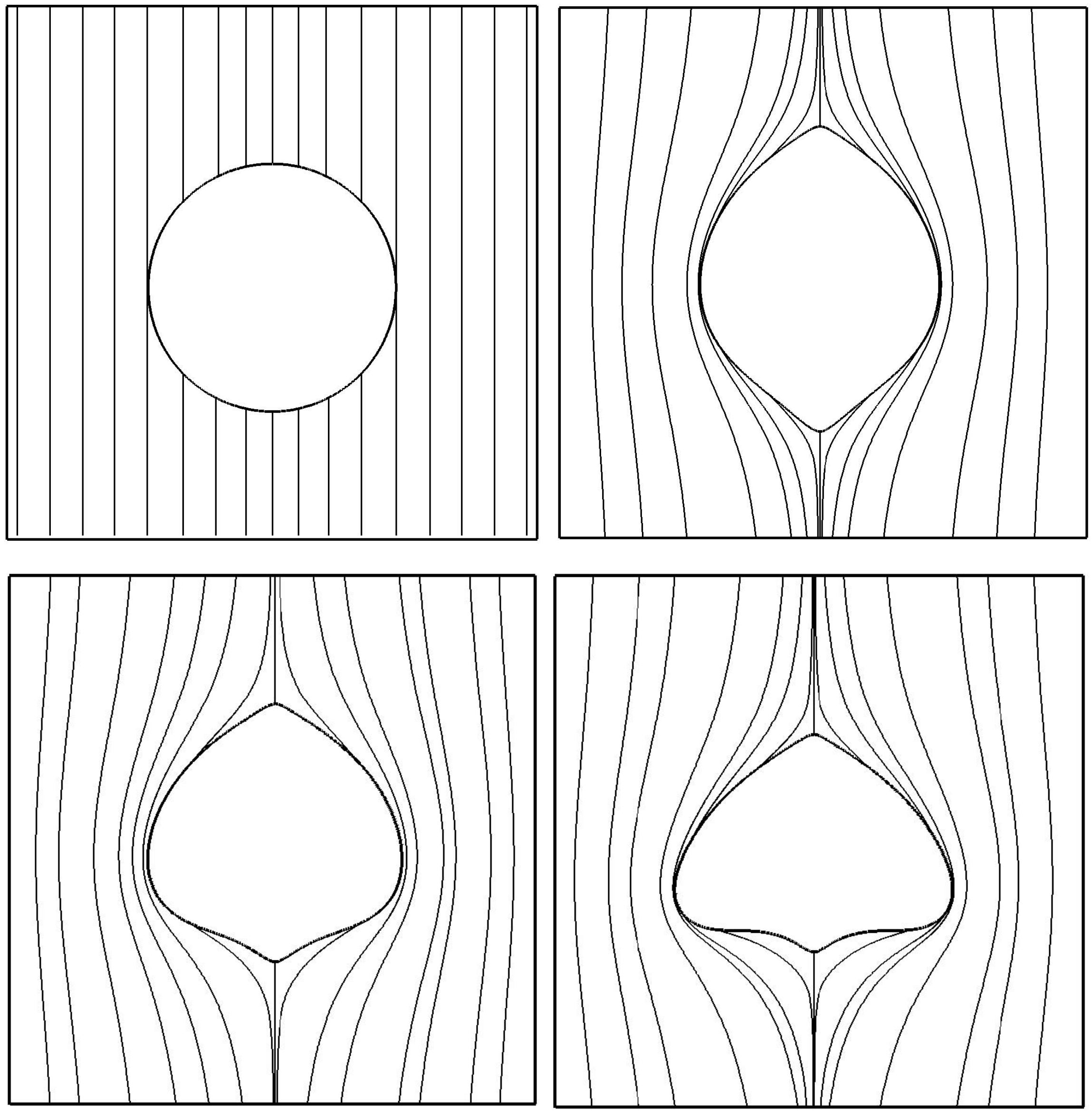


Figure 6: A Newtonian bubble rising in a nematic fluid (Zhou, Feng, Yue, Liu & S. '07)

Nematic liquid crystal drops in a Newtonian matrix under simple shear

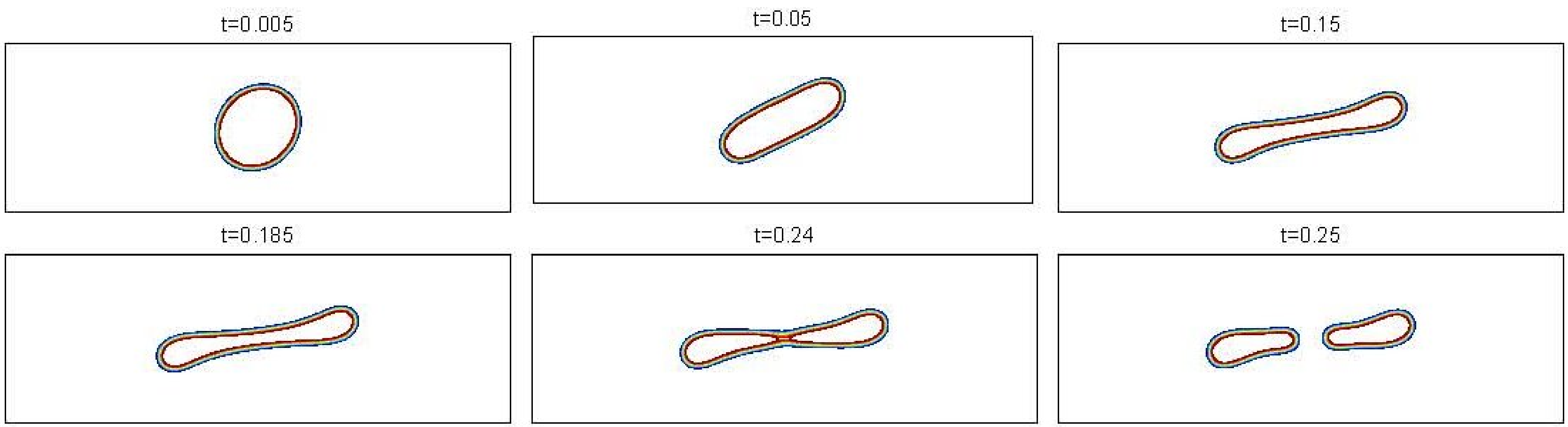


Figure 7: Newtonian drop in a Newtonian matrix: Cahn-Hilliard phase equation

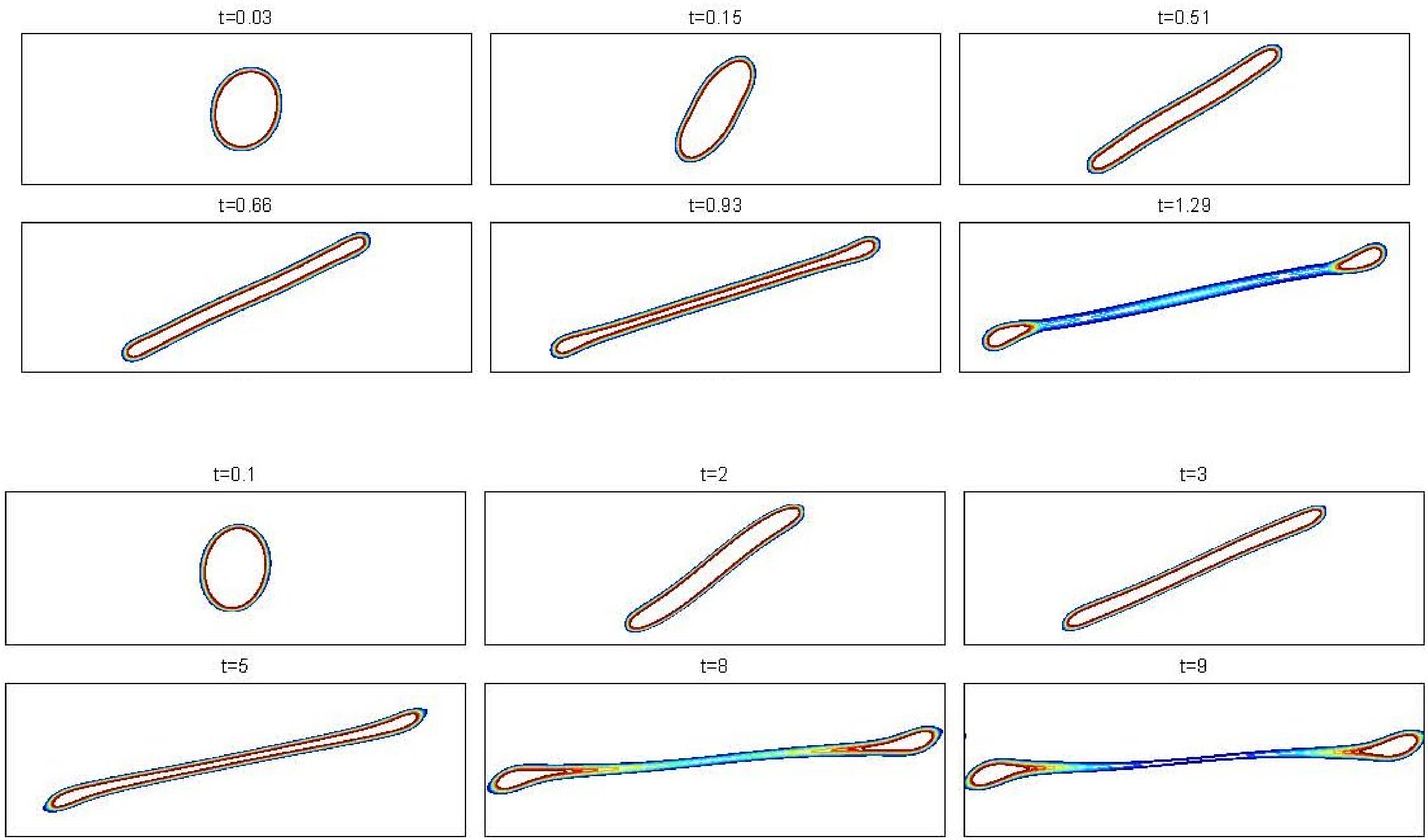
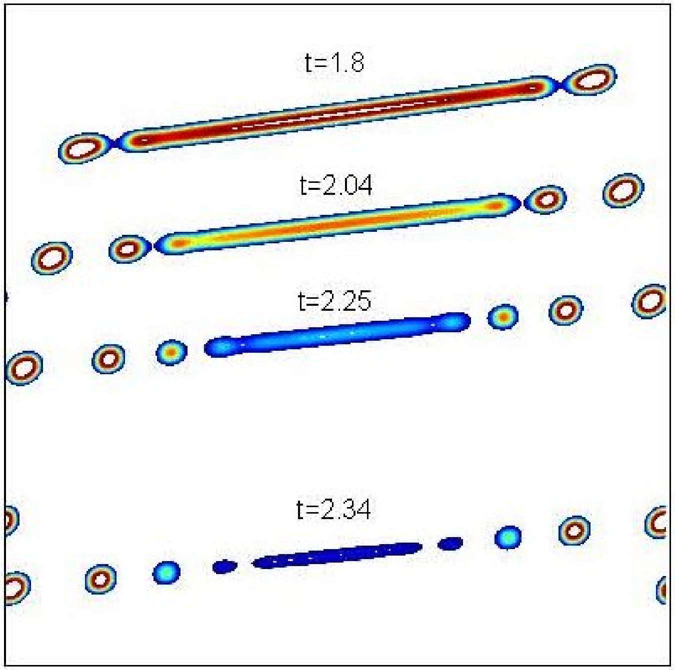


Figure 8: Liquid crystal drop in a Newtonian matrix: Top, Cahn-Hilliard; bottom: Allen-Cahn



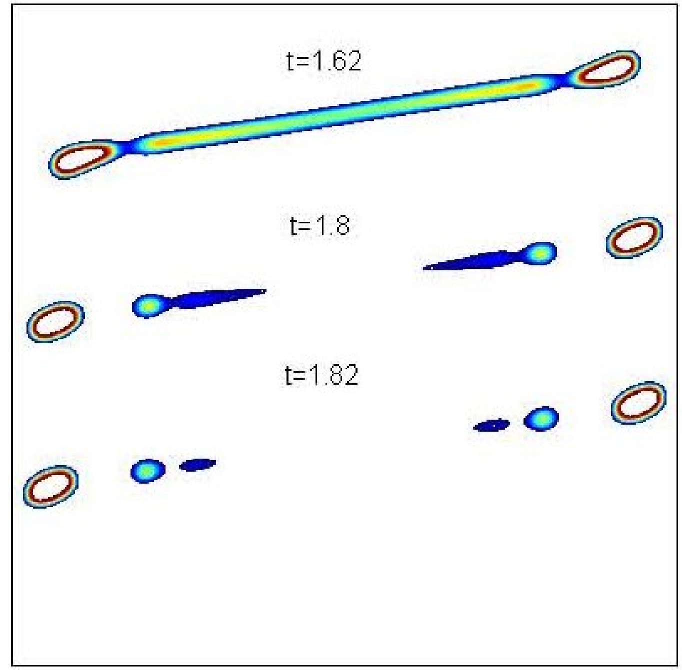


Figure 9: Liquid crystal drop in a Newtonian matrix (Cahn-Hilliard): left figure with larger viscosity

Concluding remarks

- The mixture of two incompressible fluids can be described by a flexible and robust energetic phase field model.

- An alternative phase-field model based on the density is proposed: it is particularly suitable for problems with large density ratios and it admits an energy law.

- Some efficient numerical approaches for solving the coupled system are proposed:
  - a stablized semi-implicit scheme for the phase equation;

– new projection type schemes which only require solving regular Poisson equation for the pressure;
– a moving mesh spectral discretization in space.

Advantages and challenges:

- The proposed numerical schemes are easy to implement as they are all based only on elliptic solves with regular Poisson equation for the pressure.

- It can be easily extended to handle some non-Newtonian flows such as liquid crystal flows and visco-elastic flows, ...

- It is possible to treat multiphase (> 2) flows by introducing multiple phase functions.

- Treating all nonlinear terms explicitly lead to a somewhat restrictive time step constraint. We are currently working on ways to **efficiently** treat some nonlinear terms implicitly to improve the stability.

Thank you!