On the Influence of Surfactants on the Wake and Shape of Gaseous Bubbles Ascending in Liquids

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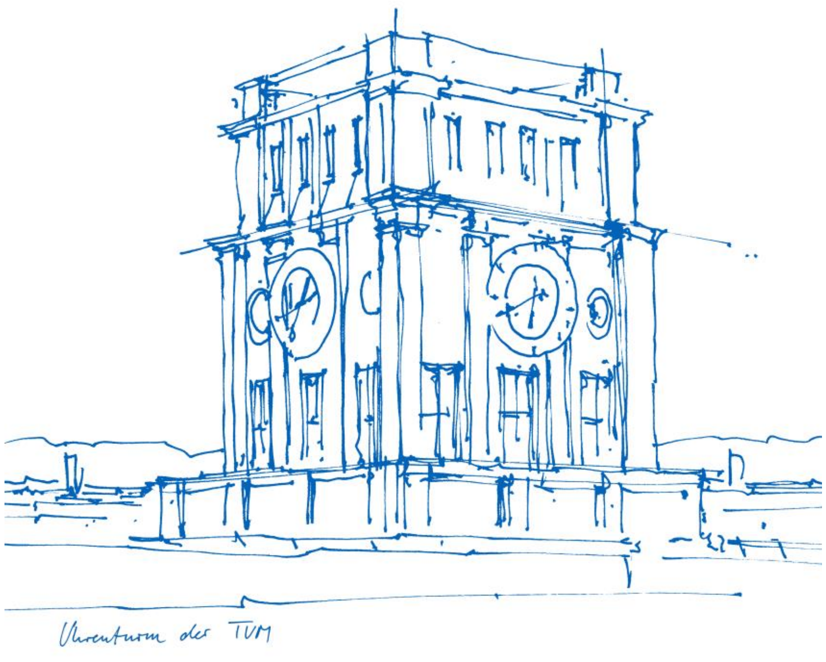
Firenze, Italy, 23.05.2016



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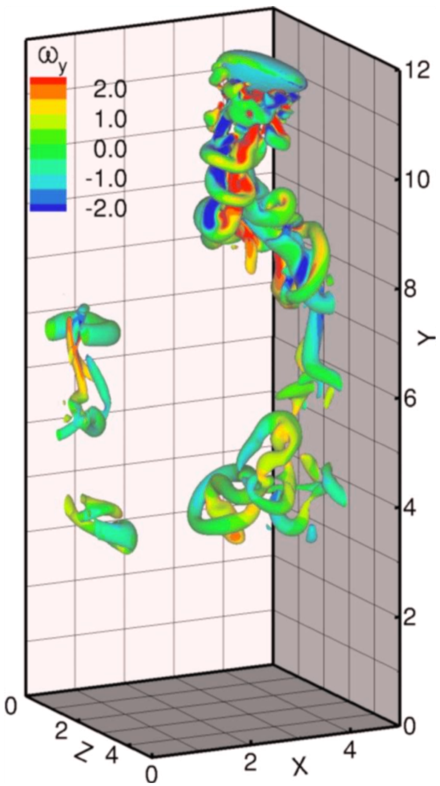
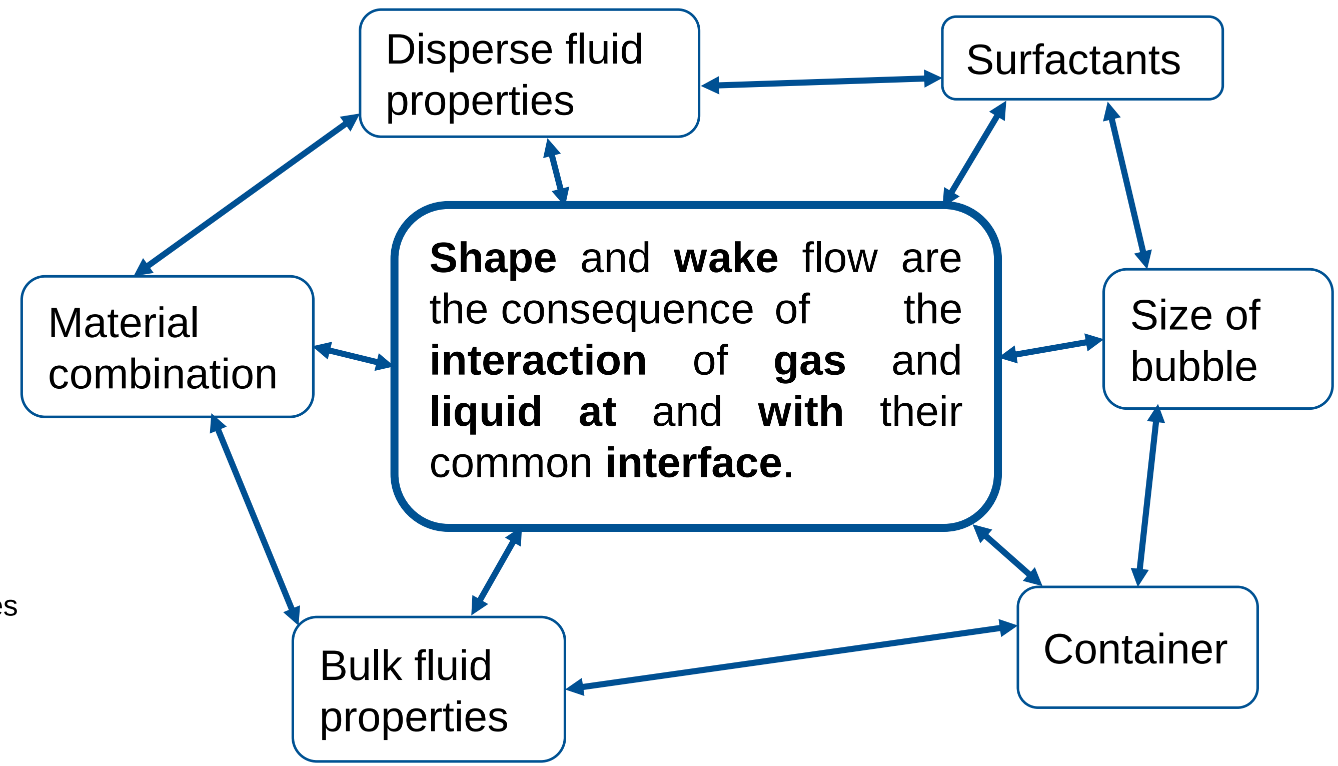
Motivation



Bubble with wake. Vortex structures are visualized using the isosurface $\lambda_2 = -0.2$; coloured with vertical vorticity ω_y[1].

General interest:

- Bubble induced vorticity improves mixing and homogenization of the bulk phase [1]
  → Process engineering



[1]:D.Gaudlitz, N. Adams; *Numerical investigation of rising bubble wake and shape variations*; Physics of Fluids; 21; 2009

Aim of this Study:

Employ

- ► A physically consistent method for underresolved simulations of weakly compressible flows (iLES)
- ► Weakly Compressible Sharp-Interface Method [*]
- ► Conservative Interface-Interaction Model with Insoluble Surfactant Dynamics [+,#]

Study

- Influence of surfactant on the shape and (wake) of bubbles ascending in a denser liquid
- Dynamic redistribution of surfactant

→ **Guidelines for**

- Numerical modeling
- Controlling bubble shape and wake via surfactant parameters

[*]: F.Schranner,N.Adams, *A Conservative Interface-Interaction Model with Insoluble Surfactant*, suggested for publication to the Journal of Computational Physics
[+]: F.Schranner, X.Hu, N.Adams, *On the Convergence of the Weakly Compressible Sharp-Interface Method for Two-Phase Flows*, suggested for publication to the Journal of Computational Physics
[#]: J.Luo, X.Hu, N.Adams, *A conservative sharp interface method for incompressible multiphase flows*, Journal of Computational Physics 284, 2015, pp. 547-565

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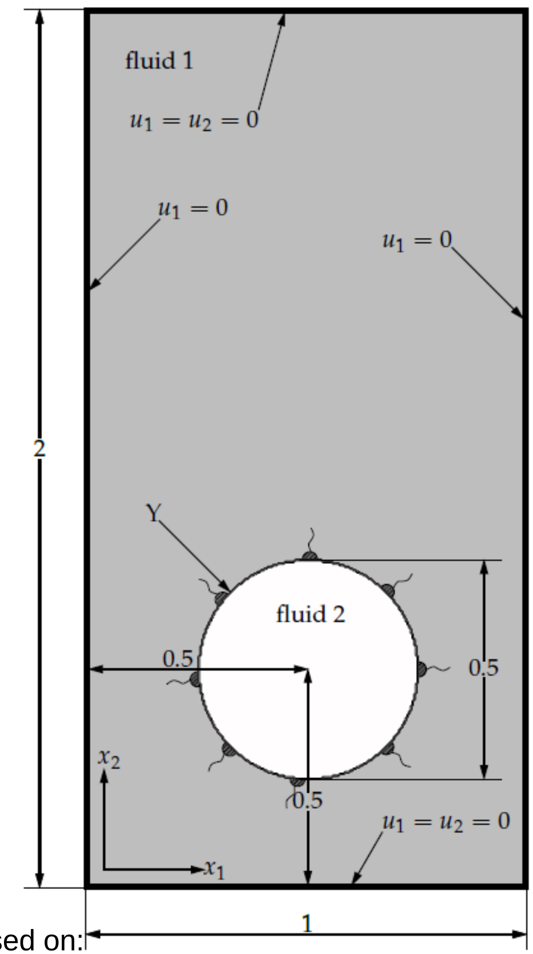
Setup



Grid: 256x512 Finite volumes

→ 128 Cells across bubble

Relative errors (circularity & velocity):

$\|e_1\|, \|e_2\|, \|e_\infty\| \sim 10^{-3}$

Interfacial γ-Diffusion considered

$$Pe_s^* = \frac{U_{ref} d_{ref}}{D_s} = 10$$

$$D_s = 0.035 \, \frac{m^2}{s}$$

Setup based on:
S. Hysing, S. Turek, D. Kuzmin, N. Parolini, E. Burman, S. Ganesan, L. Tobiska; *Quantitative benchmark computations of two-dimensional bubble dynamics*; International Journal for Numerical Methods in Fluids 60 (11) (2009) 1259-1288

Test cases:

Case 2:

$\sigma_0 = 24.5 \frac{N}{m}, \quad \mu_{ref} = 10 \frac{kg}{ms}$

$\Delta\rho = 900 \frac{kg}{m^3}, \frac{\mu_{ref}}{\mu_b} = 10$

$\rho_{ref} = 1000 \frac{kg}{m^3}, \frac{\rho_{ref}}{\rho_b} = 10$

$\rightarrow Re^* = 35$

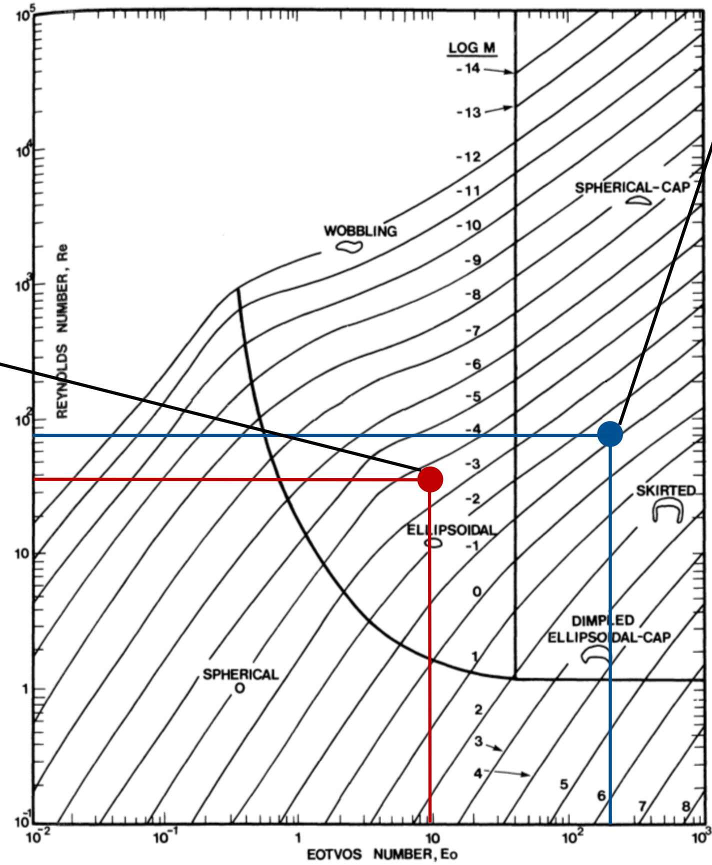
$\rightarrow Eo = 9$

$\rightarrow log(Mo) \approx -3.2$

→ Ellipsoidal

$$Re^* = \frac{U_{ref} d_{ref} \rho_{ref}}{\mu_{ref}},$$

$$Eo = \frac{\Delta\rho\, g\, d_{ref}^2}{\sigma_0}, \quad Mo = \frac{g\, \mu_{ref}^4 \Delta\rho}{\sigma_0^3 \rho_{ref}^2}$$



Bubble shapes and regimes for free buoyancy driven ascent in liquids. Adopted from [2].

Case 1:

$\sigma_0 = 1.225 \frac{N}{m},$

$\mu_{ref} = 3.5 \frac{kg}{ms}, \frac{\mu_{ref}}{\mu_b} = 100$

$\Delta\rho = 999 \frac{kg}{m^3},$

$\rho_{ref} = 1000 \frac{kg}{m^3}, \frac{\rho_{ref}}{\rho_b} = 1000$

$\rightarrow Re^* = 100$

$\rightarrow Eo = 200$

$\rightarrow log(Mo) \approx -1.1$

→ Skirted-Cap

[2]: R.Clift, J.Grace, M.Weber, *Bubbles, Drops, and Particles*, Dover Publications, Inc., Mineola, New York, USA, 2005

What are we studying?

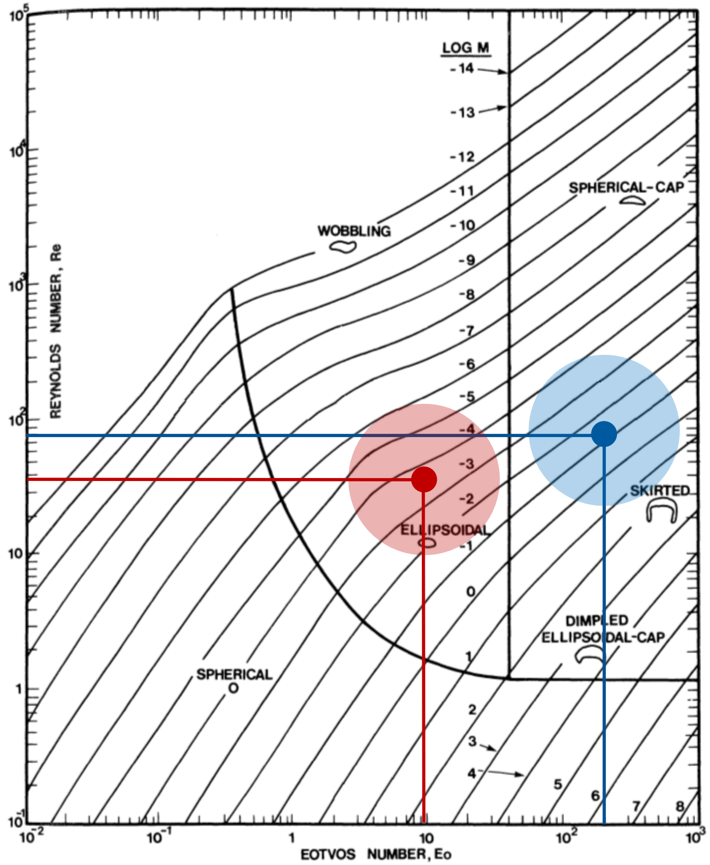
Surfacant parameters:

$\zeta = \frac{\gamma_{eq}}{\gamma_\infty}$: coverage

$\beta = \frac{RT\gamma_\infty}{\sigma_0}$: Elasticity

with:

$$\gamma_{eq} = \frac{1}{\Delta\Upsilon}\int_{\Delta\Upsilon}\gamma d\ \Upsilon'\bigg|_{t=0}$$



Bubble shapes and regimes for free buoyancy driven ascent in liquids. Adopted from [2].

Equation of state(EoS):

non-linear Langmuir EoS:

$$\sigma = \sigma_0(1 + \beta\ ln(1 - \zeta\,\gamma))$$

linear Langmuir EoS:

$$\sigma = \sigma_0(1 - \beta\,\zeta\,\gamma)$$

[2]: R.Clift, J.Grace, M.Weber, *Bubbles, Drops, and Particles*, Dover Publications, Inc., Mineola, New York, USA, 2005

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Case 1

$$\boxed{\zeta = \frac{\gamma_{eq}}{\gamma_\infty}}$$

$Re^* = 100$

$Eo = 200$

$log(Mo) \approx -1.1$

$\beta = 0.3$

non-lin-EoS:

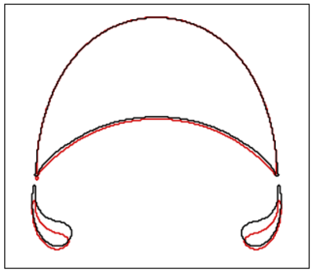
$\sigma = \sigma_0(1 + \beta\ ln(1 - \zeta\gamma))$

$\zeta = 0.1\ - nonlin$

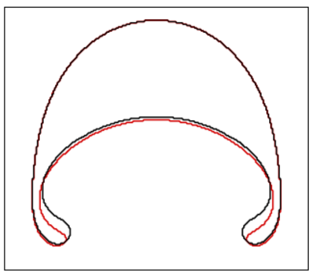
$\zeta = 0.6\ - nonlin$

$\zeta = 0.1\ - lin$

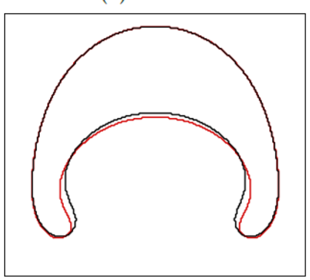
$\zeta = 0.6\ - lin$



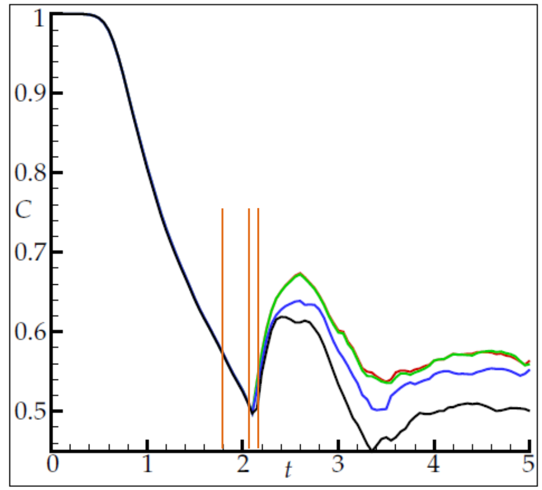
(c) $t = 2.15$



(b) $t = 2.05$



(a) $t = 1.8$



(a) Degree of circularity C

- Small ζ lin. ≈ ζ non-lin
- Large ζ nonlin ≠ ζ lin
- Large ζ lin EoS ≈ small ζ/ ζ

- Larger ζ non-lin EoS
  → Smaller circularity
  → Larger secondary bubbles

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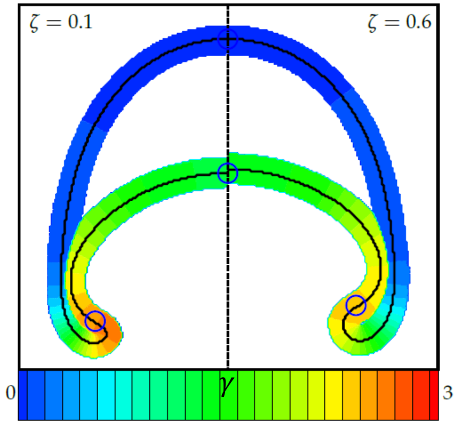
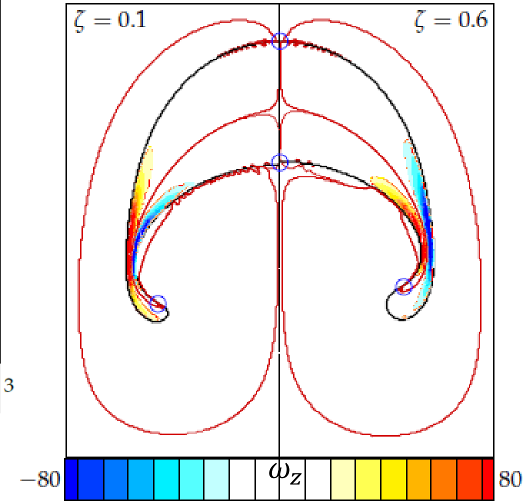
Case 1

$$\boxed{\zeta = \frac{\gamma_{eq}}{\gamma_\infty}}$$

$$Re^* = 100$$
$$Eo = 200$$
$$log(Mo) \approx -1.1$$
$$\beta = 0.3$$



(c) $t = 2.05$, non-linear



(c) $t = 2.05$, non-linear

- Surfactant travels to and accumulates at the zero vorticity points
- Overlap of $\omega_z = 0$ and interface
  → $\nabla\gamma$ small
- Large ζ
  → $\nabla\gamma$ smaller (uniformity higher)
  → Lower γ at outer zero vorticity points
  → Lower $|\omega_z|$

Case 1

$\boxed{\beta}$

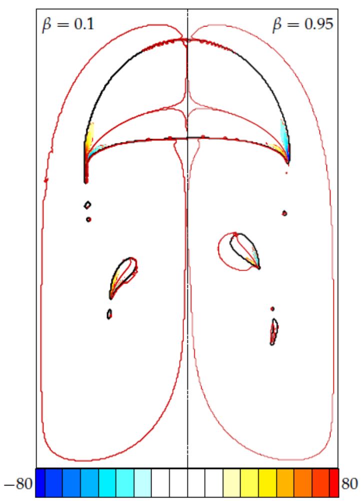
$$Re^* = 100$$
$$Eo = 200$$
$$log(Mo) \approx -1.1$$
$$\zeta = 0.3$$

- Larger secondary bubbles
  → Lower Circularity
  → Larger ascent velocity

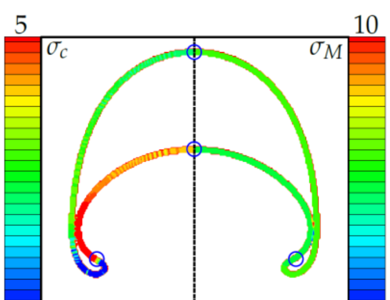
Similar to increasing ζ

- Larger β
  → Decrease of curvature
  → Larger secondary bubbles
  → more surfactant remains with mother bubble

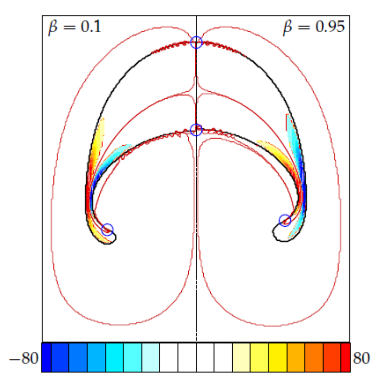
- Less tip-streaming



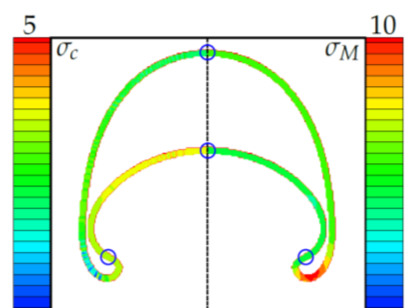
(e) $t = 3.6$, non-linear



(f) $t = 2.05$, non-linear, $\beta = 0.1$



(c) $t = 2.05$, non-linear



(e) $t = 2.05$, non-linear, $\beta = 0.95$

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Case 2

$$\boxed{\zeta = \frac{\gamma_{eq}}{\gamma_\infty}}$$

non-lin-EoS:

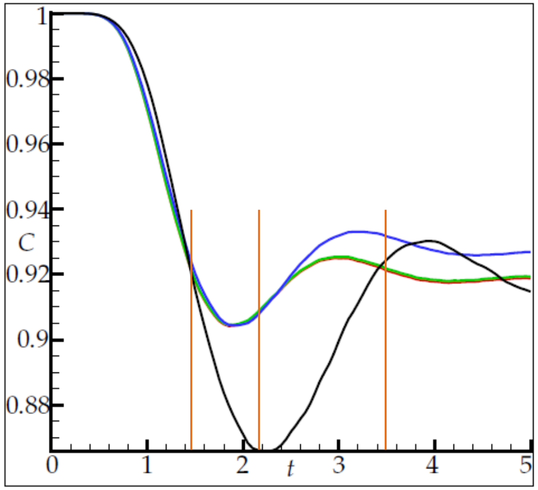
$$\sigma = \sigma_0(1 + E\ ln(1 - \zeta\gamma))$$

$\zeta = 0.1\ - nonlin$

$\zeta = 0.6\ - nonlin$

$\zeta = 0.1\ - lin$

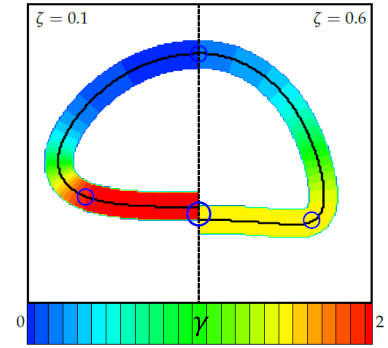
$\zeta = 0.6\ - lin$



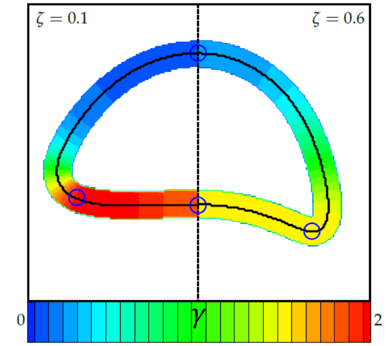
(a) Degree of circularity C

- Small ζ lin. ≈ ζ non-lin
- Large ζ lin EoS ≠ ζ non-lin

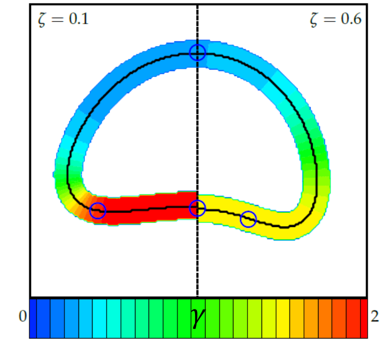
- γ redistribution completed quickly
- Small ζ : γ higher at stern
- Large ζ : γ distributes along flanks



(e) $t = 3.5$, non-linear



(c) $t = 2.15$, non-linear



(a) $t = 1.45$, non-linear

$$Re^* = 35$$
$$Eo = 9$$
$$log(Mo) \approx -3.2$$
$$\beta = 0.3$$

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$$Re^* = 35$$
$$Eo = 9$$
$$log(Mo) \approx -3.2$$
$$\beta = 0.3$$

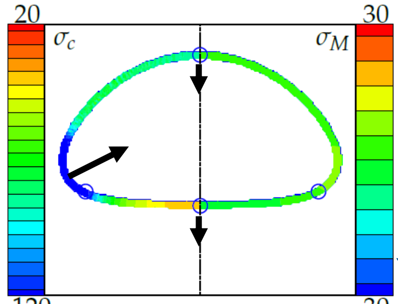
Case 2

$\zeta = 0.1\ - nonlin$

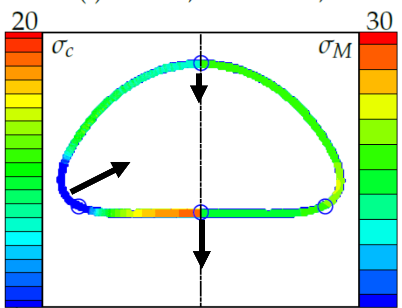
$\zeta = 0.6\ - nonlin$

Arrows: Stresses as acting on interface
Colour: Mathematical orientation

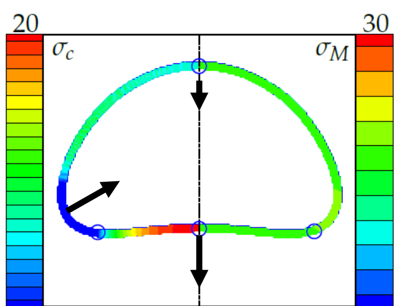
- ▶ Stress balance
- ▶ Terminal shape
- ▶ Terminal velocity



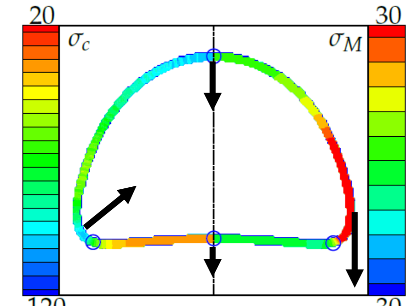
(i) $t = 3.5$, non-linear,



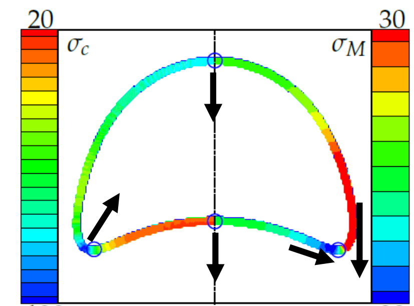
(f) $t = 2.15$, non-linear,



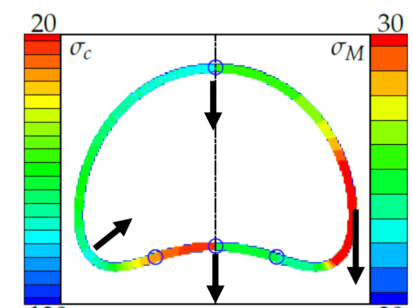
(c) $t = 1.45$, non-linear, $\zeta = 0.1$



(h) $t = 3.5$, non-linear,



(e) $t = 2.15$, non-linear,



(b) $t = 1.45$, non-linear, $\zeta = 0.6$

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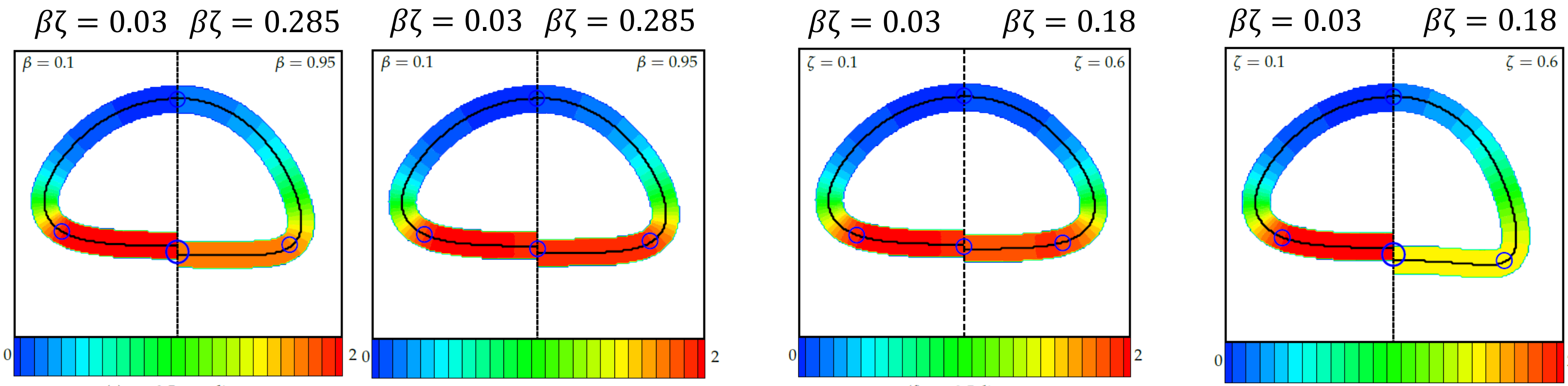
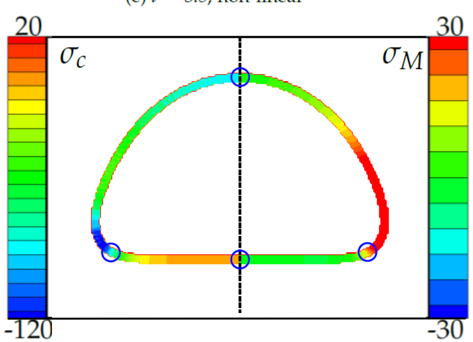
Case 2

$\boxed{\beta}$

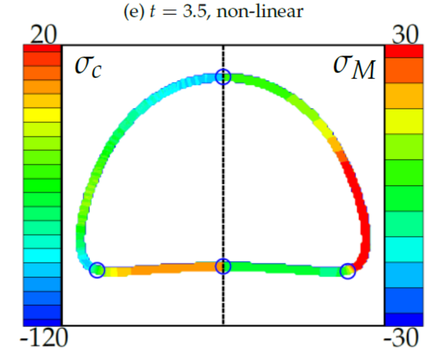
$$Re^* = 35$$
$$Eo = 9$$
$$log(Mo) \approx -3.2$$



(e) $t = 3.5$, non-linear (f) $t = 3.5$, linear (f) $t = 3.5$, linear (e) $t = 3.5$, non-linear



- ▶ Increase of $\beta\zeta$
  - → $\omega_z = 0$ outwards
- ▶ Effect of ζ on σ stronger as β
  - → Stronger elongation
  - → Slower bubble
  - → Lower γ at stern



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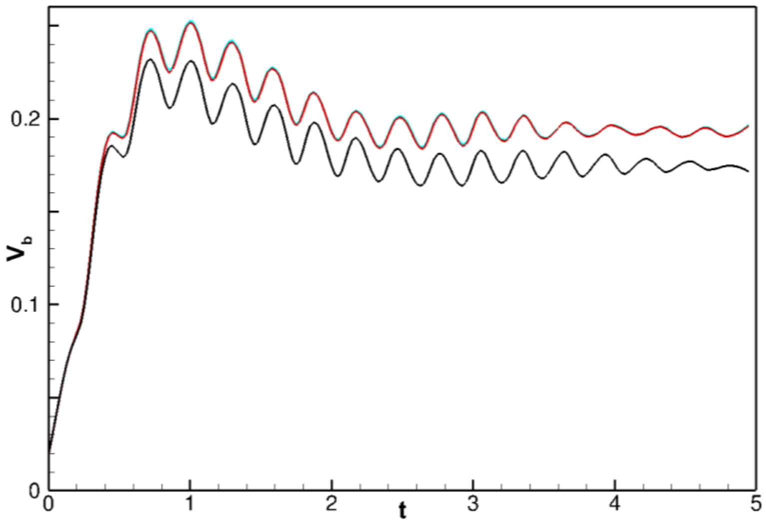
Case 2



$\zeta = 0.1 \ - nonlin$

$\zeta = 0.6 \ - nonlin$

$clean$

Note on Case 1:
No effect on terminal ascent velocity

In agreement with e.g.:

- Savas Tasoglu, Utkan Demirci and Metin Muradoglu; *The effect of soluble surfactant on the transient motion of a buoyancy-driven bubble;* Physics of Fluids 20, 2008
- Tryggvason, Brunner, Esmaeeli; *Front-Tracking Method for the Computations of Multiphase Flow*; Journal of Computation Physics; 2001
- N. M. Aybers, A. Tapucu; *The motion of gas bubbles rising through stagnant liquid*, Wärme - und Stoffübertragung 2;1969
- A. Brankovic, I. Currie, W. Martin, *Laser-Doppler measurements of bubble dynamics*, Physics of Fluids 27; 1984
- F. Durst, B. Schnung, K. Selanger, M. Winter, *Bubble-driven liquid flows*, Journal of Fluid Mechanics 170; 1986

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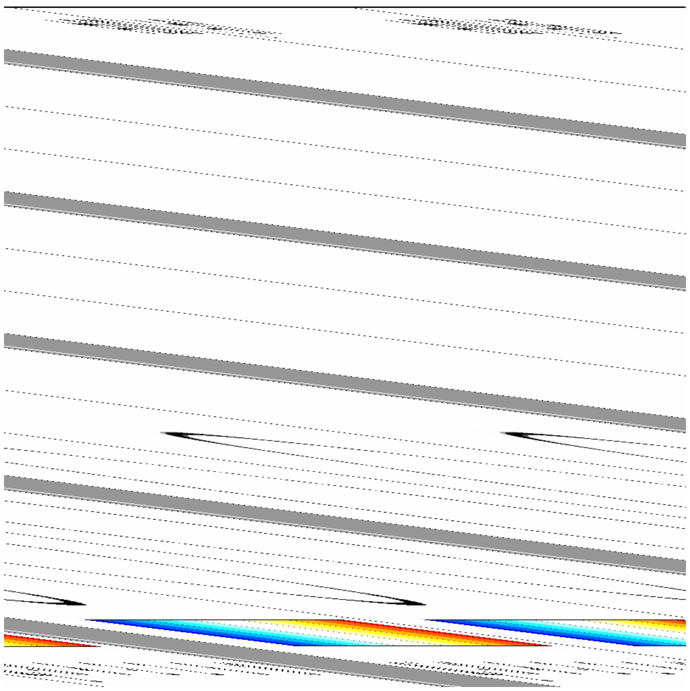
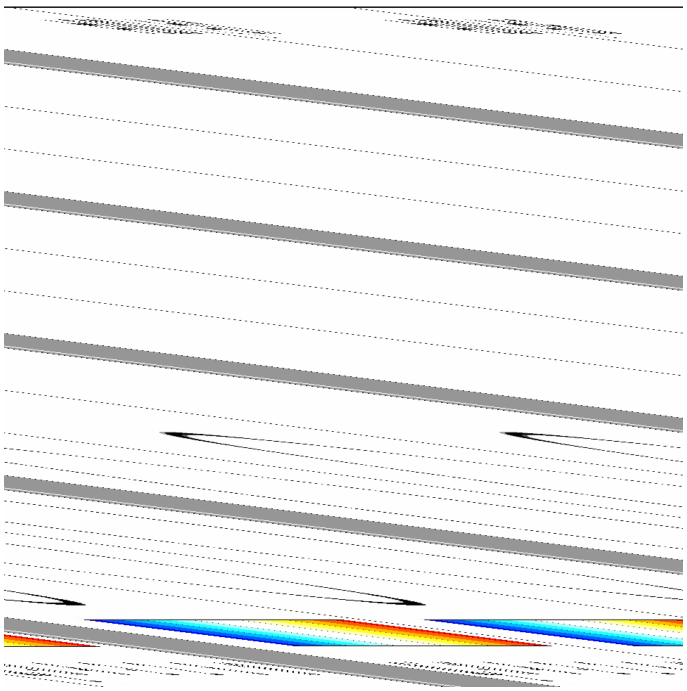
Case 2

Vorticity concentrates in the lighter phase [3]

Case 1





[3]:M.K.Triphati,K.C.Sahu,R.Govindarajan; *Why a falling drop does not in general behave like a rising bubble*; Scientific Reports; 4, 2014

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Case 2

$$C_d = \frac{4}{3}\frac{\Delta\rho g d_{ref}}{\rho_{ref} V_b^2} \quad [4]$$

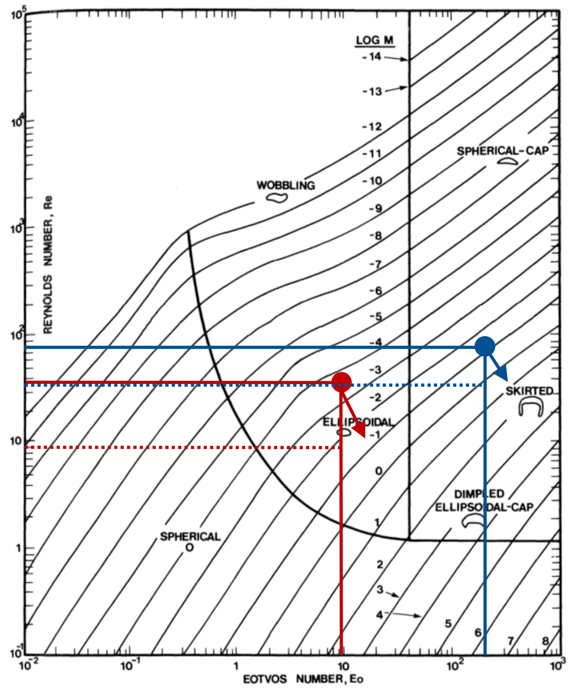
Case 1

Case 2:

$Eo = 9$

$log(Mo) \approx -3.2$

ζ	β	C_d	Re
0	0	15.79	9.5
0.1	0.3	17.05	9.29
0.6	0.3	21.53	8.27
0.3	0.1	17.00	9.30
0.3	0.95	21.73	8.23



Bubble shapes and regimes for free buoyancy driven ascent in liquids. Adopted from [2].

Case 1:

$Eo = 200$

$log(Mo) \approx -1.1$

ζ	β	C_d	Re
0	0	12.58	32.85
0.1	0.3	11.65	33.81
0.6	0.3	11.33	34.28
0.3	0.1	11.67	33.71
0.3	0.95	12.66	32.43

→Increasing *β / ζ stronger effect on C_d for Case 2*

[2]: R.Clift, J.Grace, M.Weber, *Bubbles, Drops, and Particles*, Dover Publications, Inc., Mineola, New York, USA, 2005

[4]:Y. J. Yan; *Computational studies of bubble dynamics*; Ph.D. thesis, The University of Michigan, 1994

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Key findings of this study

- ► Surfactant travels to and accumulates at the zero vorticity points [5]
  → Can be confirmed qualitatively

- ► Effect of surfactant is strong for bubbles of smaller Eo, for large Eo, effect is almost negligible [6,7].
  → Can be confirmed qualitatively

Key Findings

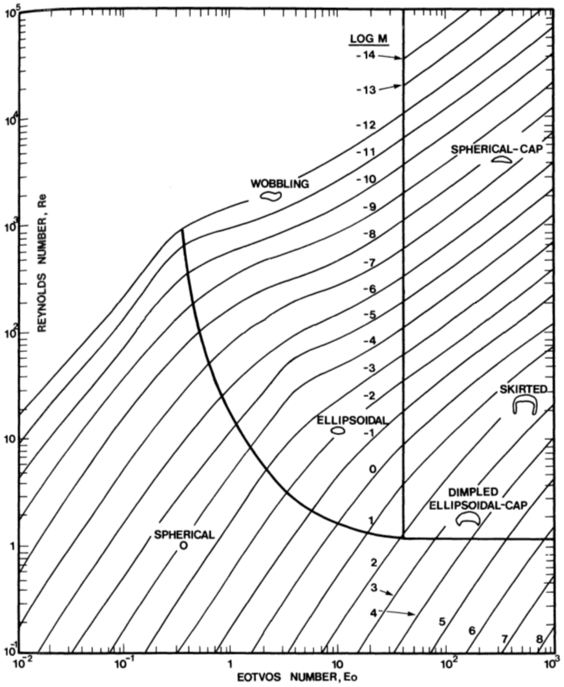
- ► Surfactant can shift vorticity concentration from less dense phase to dense phase [3]

- ► Non-linear Langmuir EoS applicable

[5]: Y. Tseng, A. Prosperetti; *Local interfacial stability near a zero vorticity point;* Journal of Fluid Mechanic 776; 2015
[6]: P. C. Duineveld, *The rise velocity and shape of bubbles in pure water at high Reynolds number*, Journal of Fluid Mechanics 292; 1995
[7]: R. Hartunian, W. Sears, *On the instability of small gas bubbles moving uniformly in various liquids*, Journal of Fluid Mechanics 3; 1957
[3]: M.K.Triphati,K.C.Sahu,R.Govindarajan; *Why a falling drop does not in general behave like a rising bubble*; Scientific Reports 4; 2014

Outlook/Ongoing

- Disregard interfacial γ-diffusion (Realistically: $D_s \approx 10^{-9}\frac{m^2}{s}$)
- Continue with non-linear EoS
- Full parameter study (β,ζ)
- Find saturation (β,ζ)
- Extend analysis to smaller Morton, for $Eo \leq 20$ [7].



Bubble shapes and regimes for free buoyancy driven ascent in liquids. Adopted from [2].

[7]: Savas Tasoglu, Utkan Demirci and Metin Muradoglu; *The effect of soluble surfactant on the transient motion of a buoyancy-driven bubble;* Physics of Fluids 20, 2008 → $Eo \approx 20$ *is boundary for effect of* γ

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Acknowledgements:

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Computational resources: Munich Centre of Advanced Computing (MAC)

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What are we studying?

Case 2:

$$\sigma_0 = 24.5 \frac{N}{m}$$

$$\mu_{ref} = 10 \frac{kg}{ms}$$

$$\Delta\rho = 900 \frac{kg}{m^3}$$

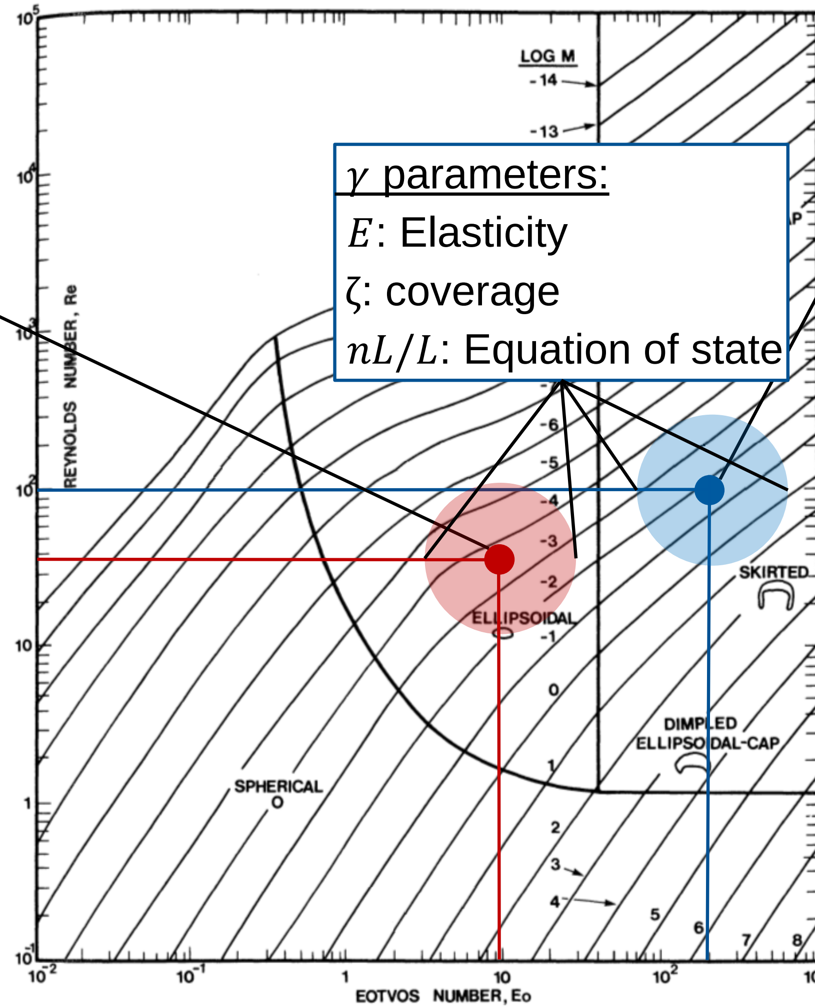
$$\rho_{ref} = 1000 \frac{kg}{m^3}$$

$\rightarrow Re = 35$

$\rightarrow Eo = 9$

$\rightarrow log(Mo) \approx -3.2$

→ Ellipsoidal



γ parameters:

E: Elasticity

ζ: coverage

nL/L: Equation of state

Bubble shapes and regimes for free buoyancy driven ascent in liquids. Adopted from [6].

Case 1:

$$\sigma_0 = 1.225 \frac{N}{m}$$

$$\mu_{ref} = 3.5 \frac{kg}{ms}$$

$$\Delta\rho = 999 \frac{kg}{m^3}$$

$$\rho_{ref} = 1000 \frac{kg}{m^3}$$

$\rightarrow Re = 100$

$\rightarrow Eo = 200$

$\rightarrow log(Mo) \approx -1.1$

→ Skirted-Cap

[6]: R.Clift, J.Grace, M.Weber, *Bubbles, Drops, and Particles*, Dover Publications, Inc., Mineola, New York, USA, 2005

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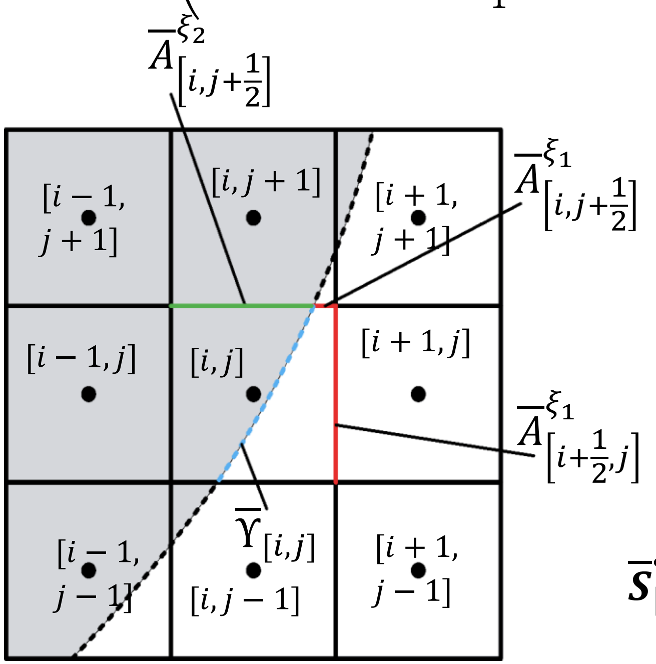
Numerical Method I

$$\widetilde{\boldsymbol{U}}^{\xi_i,n+1}_{[i,j]} = \widetilde{\boldsymbol{U}}^{\xi_i,n}_{[i,j]} + \Delta t \boldsymbol{L}^{\xi_i,n}_{[i,j]}$$

$$\boldsymbol{L}^{\xi_i,n}_{[i,j]} = \left(\frac{\left[\overline{A}\,\overline{\boldsymbol{F}}_1\right]^{\xi_i}_{[i-1/2,j]} - \left[\overline{A}\,\overline{\boldsymbol{F}}_1\right]^{\xi_i}_{[i+1/2,j]}}{\Delta x_1} + \frac{\left[\overline{A}\,\overline{\boldsymbol{F}}_2\right]^{\xi_i}_{[i,j-1/2]} - \left[\overline{A}\,\overline{\boldsymbol{F}}_2\right]^{\xi_i}_{[i,j+1/2]}}{\Delta x_2} + \overline{\boldsymbol{S}}^{\xi_i}_{[i,j]} + \frac{\overline{\boldsymbol{X}}^{\xi_i}_{[i,j]}}{\Delta V_{[i,j]}} \right)$$



$$\widetilde{\boldsymbol{U}}^{\xi_i}_{[i,j]} = \left\{\zeta\, \widehat{\boldsymbol{U}}\right\}^{\xi_i}_{[i,j]} \qquad \zeta^{\xi_i}{}_{[i,j]} = \left.\frac{\Delta V^{\xi_i}}{\Delta V}\right|_{[i,j]}$$

$$\widehat{\boldsymbol{U}}^{\xi_i}_{[i,j]} = \frac{1}{\Delta V_{[i,j]}} \int_{\Delta V_{[i,j]}} \boldsymbol{U}^{\xi_i}_{[i,j]} dV'$$

Interface fluxes:

$$\overline{\boldsymbol{X}}^{\xi_i}_{[i,j]} = \left\{\overline{\boldsymbol{X}}^{\perp} + \overline{\boldsymbol{X}}^{\parallel}\right\}^{\xi_i}_{[i,j]}$$

Note: $\overline{*} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} * \, dt$

$$\overline{\boldsymbol{S}}^{\xi_i}_{[i,j]} = \frac{1}{Fr^2} \left(\overline{\rho}^{\xi_i}_{[i,j]} - 1\right) \begin{bmatrix} 0 \\ 0 \\ -g \end{bmatrix}^T$$

Intercell numerical fluxes:

$F_{1,[i\pm1/2,j]}, F_{2,[i,j\pm1/2]}$

adv. Flx.: Roe Riemann flux & WC-WENO-CU6-M1[7]

Visc. Flx: 4th- order accurate

[7] F.Schranner,V.Rozov,N.Adams,*Optimization of an Implicit Large-Eddy Simulation Method for Underresolved Incompressible Flow Simulations*, AIAA-Journal, 54, 5, 2016

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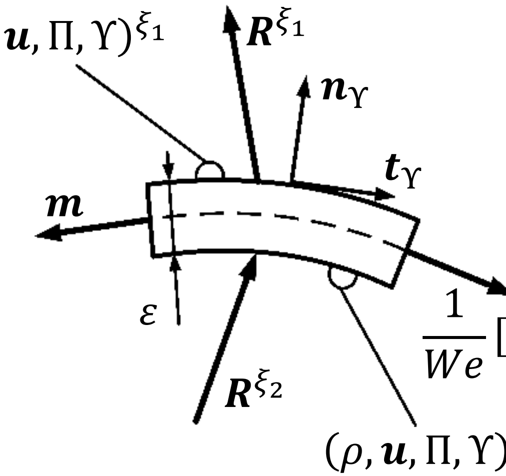
Numerical Method II

Interface fluxes:

$$\overline{\boldsymbol{X}}^{\xi_i}_{[i,j]} = \left\{\overline{\boldsymbol{X}}^{\perp} + \overline{\boldsymbol{X}}^{\parallel}\right\}^{\xi_i}_{[i,j]}$$

$$\left\{r^{\xi_i}_{\Upsilon,\perp}\Upsilon\begin{bmatrix}0\\ \boldsymbol{n}^{\xi_i}_{\Upsilon}\end{bmatrix}\right\}_{[i,j]} \qquad \left\{r^{\xi_i}_{\Upsilon,\parallel}\Upsilon\begin{bmatrix}0\\ \boldsymbol{t}_{\Upsilon}\end{bmatrix}\right\}_{[i,j]}$$



$$\frac{1}{We}\oint_s \boldsymbol{m}\, ds' = \frac{1}{We}\left[-\sigma\boldsymbol{n}_{\Upsilon}(\boldsymbol{\nabla}^T\cdot\boldsymbol{n}_{\Upsilon}) + (\nabla_{\Upsilon}\sigma)\right]\Delta\Upsilon$$

$$r^{\xi_i}_{\Upsilon,\perp} = \frac{Z^{\xi_2}\left(r^{\xi_1}_{\perp} + \sigma_c\delta_{i2}\right) + Z^{\xi_1}\left(r^{\xi_2}_{\perp} + \sigma_c\delta_{i1}\right)}{Z^{\xi_1} + Z^{\xi_2}} + \frac{Z^{\xi_1}Z^{\xi_2}\left(u^{\xi_1}_{\perp} - u^{\xi_2}_{\perp}\right)}{Z^{\xi_1} + Z^{\xi_2}}$$

$$r^{\xi_i}_{\Upsilon,\parallel} = \frac{Z^{\xi_2}\left(r^{\xi_1}_{\parallel} + \boldsymbol{t}^{\boldsymbol{T}}_{\Upsilon}\cdot\boldsymbol{\sigma}_M\,\delta_{i2}\right) + Z^{\xi_1}\left(r^{\xi_2}_{\parallel} + \boldsymbol{t}^{\boldsymbol{T}}_{\Upsilon}\cdot\boldsymbol{\sigma}_M\,\delta_{i1}\right)}{Z^{\xi_1} + Z^{\xi_2}} + \frac{Z^{\xi_1}Z^{\xi_2}\left(u^{\xi_1}_{\parallel} - u^{\xi_2}_{\parallel}\right)}{Z^{\xi_1} + Z^{\xi_2}}$$

[3]: F.Schranner,N.Adams, *A Conservative Interface-Interaction Model with Insoluble Surfactant*, suggested for publication to the Journal of Computational Physics

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Numerical Method III

Type equation here.

[3]: F.Schranner,N.Adams, *A Conservative Interface-Interaction Model with Insoluble Surfactant*, suggested for publication to the Journal of Computational Physics