Numerical simulation of incompressible flows with particle-laden interfaces

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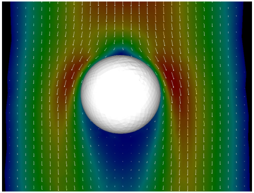
Outline

DROPS



Research focus

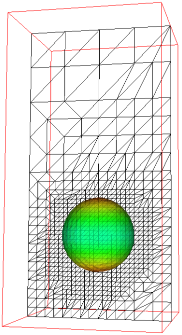
Two phase flows with transport phenomena and variable surface properties.

Methodology

- Own development; Open source (LGPL).
- Algorithms + Data structures + Post-processing.
- C++ object oriented, generic programming.
- Parallelization.

http://www.igpm.rwth-aachen.de/DROPS

Outline



- We assume that the interface is a sharp dividing surface.
- We assume the fluid to be incompressible, viscous, Newtonian, pure, and isothermal. Fluid dynamics: *Navier-Stokes* equations in separate phases.

$$\begin{cases} \rho_i \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) = \operatorname{div} \sigma_i + \rho_i \mathbf{g} \\ \operatorname{div} \mathbf{u} = 0 \end{cases}$$

with $\sigma_i = -p\mathbf{I} + \mu_i \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)$

- Standard interface condition for a clean interface:

$$[\sigma \mathbf{n}_\Gamma] = -\tau \kappa \mathbf{n}_\Gamma + \nabla_\Gamma \tau, \quad [\mathbf{u}]_\Gamma = 0,$$
$$V_\Gamma = \mathbf{u} \cdot \mathbf{n}_\Gamma$$

with V_Γ normal velocity of the interface, τ surface tension coefficient, κ curvature.

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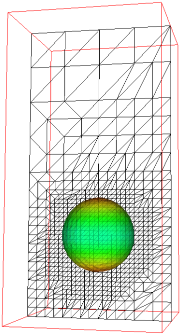
Standard model for two-phase flows



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DROPS - Key Components

- Interface condition represented as localized force term (constant τ).

$$f_\Gamma(\mathbf{v}) := -\int_\Gamma \tau\kappa\mathbf{n}\cdot\mathbf{v}\,\mathrm{d}s$$

- Level set method for interface representation.
- Finite Element methods. Extended-FEM for discontinuous quantities.
- Fast iterative solvers, multilevel techniques.
- Parallelization with MPI.

Mass Transport

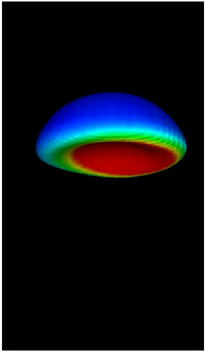
$$
\begin{aligned}
\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c &= \operatorname{div}(D_i \nabla c) && \text{in } \Omega_i, \\
[D_i \nabla c]_\Gamma \cdot \mathbf{n} = 0, \ c_1 &= C_H c_2 && \text{on } \Gamma.
\end{aligned}
$$

Henry condition : discontinuity in c. D_i: piecewise constant.

Surfactant Transport

$$
\frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S + S \operatorname{div}_\Gamma \mathbf{u} = \operatorname{div}_\Gamma (D_\Gamma \nabla_\Gamma S) \qquad \text{on } \Gamma.
$$

- τ does not depend on S.
- Observation: accumulation of surfactant at the bottom.



- For both models special numerical methods have been developed.

Outline

Surfactant versus Solid Particles

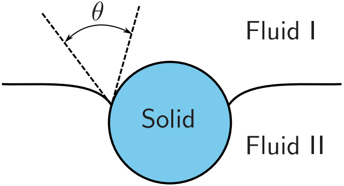
Surfactant

Surface-active materials: bipolar large molecules with hydrophobic and hydrophilic segments.

- Attracted to an interface.
- Alter interfacial tension.
- Stabilize fluid-fluid dispersions.

Solid particles

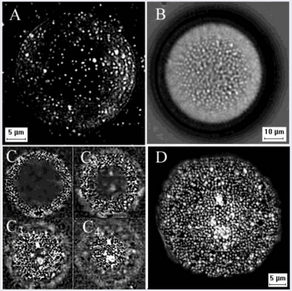
Sub-micron solid particles may also display surface activity due to three-phase equilibrium contact angle.



- Attracted to an interface.
- etc.

Complicated microscopic mechanisms and phenomena.

- Self-assembly of particles due to long range repulsive force and attractive force.
- Formation of two-dimensional structures.
- In general, adding particles at fluid interface will alter surface properties significantly.→ Applications: Emulsion stabilization (*Pickering* emulsion), health products, etc.



E. Vignati and R. Piazza, Pickering Emulsions: Interfacial Tension, Colloidal Layer Morphology, and Trapped-Particle Motion Langmuir 2003, **19**

- We investigated continuum description of surface stress tensor of the particle-laden fluid interfaces. (Macroscopic models)
- Advantage: treatment of realistic two-phase fluids.
- Challenge: choice of effective surface coefficients (e.g. viscosity).

Viscous interface model

Boussinesq-Scriven law

$$\sigma_\Gamma = [\tau + (\lambda_\Gamma - \mu_\Gamma)\,\mathrm{div}_\Gamma\, u]\mathbf{P} + 2\mu_\Gamma D_\Gamma, \quad D_\Gamma = \frac{1}{2}\mathbf{P}(\nabla_\Gamma u + \nabla_\Gamma u^T)\mathbf{P},$$

with $\mathbf{P} = \mathbf{I} - \mathbf{n}\mathbf{n}^T$ orthogonal projection, coefficients $\lambda_\Gamma, \mu_\Gamma$.

- Surface tension term.
- Dilatational viscosity term.
- Surface shear viscosity term.

Remarks

- B-S model extends the standard surface tension model ($\sigma_\Gamma = \tau\mathbf{P}$) by adding viscous terms.
- Effective viscosities are needed to model effects of nanoparticles.
- Not clear, yet, the range of systems this model is appropriate.

Treatment of general surface tension tensors

Interface stress tensor

- Standard surface tension model :

$$[\sigma \mathbf{n}_\Gamma] = -\tau\kappa\mathbf{n} + \nabla_\Gamma \tau = \mathrm{div}_\Gamma(\tau \mathbf{P}) =: \mathrm{div}(\sigma_\Gamma)$$

with σ_Γ surface stress tensor.

- General interface condition :

$$[\sigma \mathbf{n}_\Gamma] = \mathrm{div}_\Gamma(\sigma_\Gamma)$$

- Boussinesq-Scriven law :

$$\mathrm{div}_\Gamma(\sigma_\Gamma) = \mathrm{div}_\Gamma(\tau \mathbf{P} + (\lambda_\Gamma - \mu_\Gamma)\,\mathrm{div}_\Gamma\, u\, \mathbf{P} + 2\mu_\Gamma D_\Gamma)$$

Discretization of surface force

- Improved Laplace-Beltrami discretization is applied.
- Approximation quality: $\mathcal{O}(h_\Gamma)$

Choice of effective viscosities

Slattery's model

$$\sigma_\Gamma = (1 - x)\tau \mathbf{P} + 2\epsilon \mathbf{D}_\Gamma$$

where $\epsilon = Rx(\mu_1 + \mu_2)$ is the surface shear viscosity.

Lishchuk's model

$$\mu_\Gamma = \frac{5}{3}(\mu_1 + \mu_2)Rx \quad \text{surface shear viscosity}$$
$$\lambda_\Gamma = 5(\mu_1 + \mu_2)Rx \quad \text{dilatational viscosity}$$

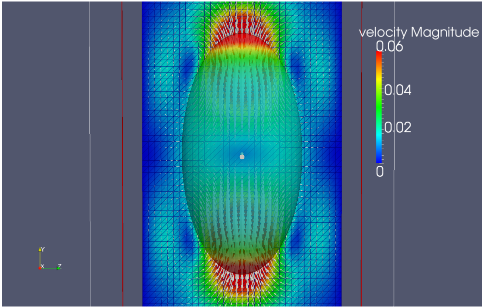
Note : R radius of particles, x coverage of particles on the interface, μ_i viscosity of bulk fluid.

Slattery, Sagis, Oh, Interfacial Transport Phenomena, 2nd Edition, Springer, 2007.
Lishchuk, Halliday, Effective Surface Viscosities of a Particle-laden Fluid Interface, Phys. Rev. E 80, 016306(2009).

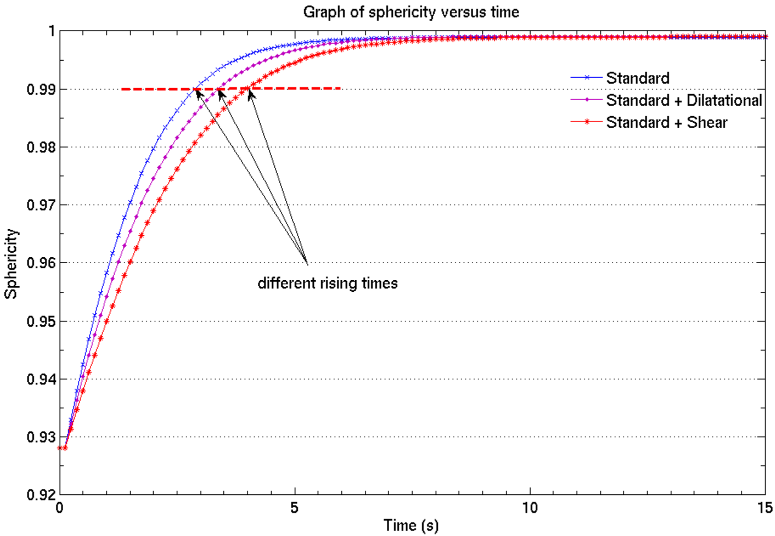
Outline

Ellipsoidal droplet

Property	Fluid I	Fluid II
ρ	1	1
μ	1	1
τ	1	
λ_Γ	1(0)	
μ_Γ	1(0)	
$\mathbf{g}$	$\mathbf{0}$	
$\mathbf{v}(0)$	$\mathbf{0}$	



Rising time



Graph of sphericity versus time
Sphericity
Time (s)
1
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0.92
0
5
10
15
Standard
Standard + Dilatational
Standard + Shear
different rising times

Outlook

- Investigation of visco-elastic interface model.
- Investigation on how to obtain effective surface coefficients.
- Improvement of iterative solver for models with viscous interface terms.
- Validation with experimental results.

More information: www.igpm.rwth-aachen.de/DROPS

- Laplace- Beltrami discretization ($\sigma_\Gamma = \tau \mathbf{P}$):

$$f_\Gamma(\mathbf{v}_h) = \tau \int_\Gamma \nabla_\Gamma \operatorname{id}_\Gamma \cdot \nabla_\Gamma \mathbf{v}_h \, ds \approx \int_{\Gamma_h} \nabla_{\Gamma_h} \operatorname{id}_{\Gamma_h} \cdot \nabla_{\Gamma_h} \mathbf{v}_h \, ds =: f_{\Gamma_h}(\mathbf{v}_h)$$

Approximation quality : $\mathcal{O}(\sqrt{h_\Gamma})$ [*S.Gross, A.Reusken, SINUM07*]

- This discretization can be improved:

$$\tilde{f}_{\Gamma_h}(\mathbf{v}_h) = \tau \int_{\Gamma_h} \tilde{\mathbf{P}}_h(\mathbf{x}) \nabla \operatorname{id}_{\Gamma_h} \cdot \nabla_{\Gamma_h} \mathbf{v}_h \, ds.$$

with $\tilde{\mathbf{n}}_h(\mathbf{x}) := \frac{\nabla \phi_h(\mathbf{x})}{\|\nabla \phi_h(\mathbf{x})\|}, \tilde{\mathbf{P}}_h(\mathbf{x}) := \mathbf{I} - \tilde{\mathbf{n}}_h(\mathbf{x})\tilde{\mathbf{n}}_h(\mathbf{x})^T$.
Approximation quality : $\mathcal{O}(h_\Gamma)$ [*S.Gross, A.Reusken, SINUM07*]

- Similar techniques has been generalized to the case with general surface tension tensor.