Numerical investigation of the interaction of two electrolytic drops under an external electric field

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Interaction of charged droplets

Drop-Interface and Drop-Drop Interactions

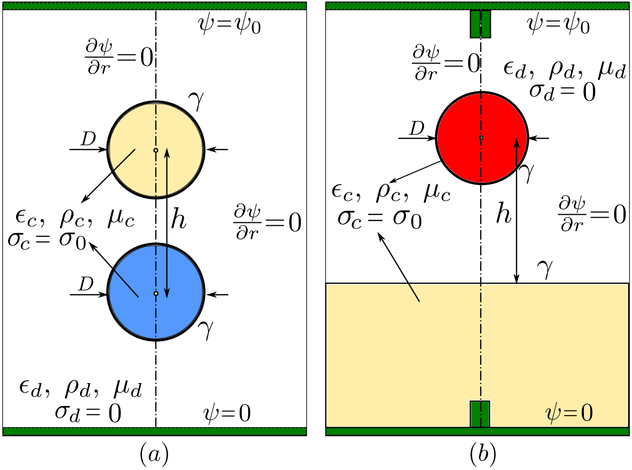


Figure: Computational domain for (a) Drop-Interface, (b) Drop-Drop interactions

Interaction of charged droplets

Codes used in the current study

- Two different numerical techniques are used
  - Finite Differences + CLSVOF method
    - Developed by my advisor and his advisor!
    - I added the charge advection using VOF
  - Finite Element + Phase field method
    - Developed by Gaute Linga
    - Based on FENICS, Code is called BERNAISE
    - `https://github.com/gautelinga/BERNAISE`

Governing equations in CLSVOF based code

- Navier-Stokes equation:
  - $\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \nabla\cdot[\mu(\nabla\mathbf{v} + \nabla\mathbf{v}^T)] + \rho\mathbf{g} + \mathbf{f}_v^\gamma + \mathbf{f}_v^E$
  - $\nabla\cdot\vec{U} = 0$
- Interface advection:
  - $\frac{\partial\phi}{\partial t} + \mathbf{v}\cdot\nabla\phi = 0$
  - $\frac{\partial F}{\partial t} + \mathbf{v}\cdot\nabla F = 0$
- Equations for quasi-electrostatics
  - $\nabla\cdot\epsilon_0\epsilon\vec{E} = q_v$
  - $\mathbf{f}_v^E = q_v\mathbf{E} - \frac{1}{2}\epsilon_0 E^2\nabla\epsilon$
  - $\frac{\partial q_v}{\partial t} + \mathbf{v}\cdot\nabla q_v + \nabla\cdot\sigma\mathbf{E} = 0$
- Surface tension forces
  - $\mathbf{f}_v^\gamma = \gamma\kappa\hat{n}\delta_s$
  - $\hat{n} = -\frac{\nabla\phi}{|\nabla\phi|}$

Numerical Schemes in CLSVOF based code

Discretization summary

- **Grid**: Staggered grid, (Harlow and Welch).
- **Viscous terms**: Second order accurate central difference scheme.
- **Convective terms**: Second order ENO scheme, (Harten et al.).
- **Surface tension**: Continuum surface force model, (Brackbill et al).
- **Electric forces**: Continuum electric force model, (Tomar et al).
- **Temporal term**: First order accurate explicit Euler method.
- **Pressure**: Second order accurate Projection method, (Chorin).
- **Interface capturing**: CLSVOF algorithm, (Sussman and Puckett) .
- **Time step**: Variable time step is used:
  - **CFL criterion** : $\Delta t \leq cfl \frac{\Delta x}{u_{max}}$
  - **Viscous time scale** : $\Delta t \leq \frac{\rho \Delta x^2}{4\mu}$
  - **Capillary time scale** : $\Delta t \leq \left[\frac{(\rho_1+\rho_2)\Delta X^3}{\gamma}\right]^{\frac{1}{2}}$
  - **Charge Relaxation time scale** : $\Delta t \leq \frac{\epsilon_0 \epsilon}{\sigma}$

Governing equations in BERNAISE

Based on FENICS

- Two-phase electrokinetic flows are described by the coupled problem of solute transport, fluid flow and electrostatics
  - $\frac{\partial}{\partial t}\rho(\phi)\vec{U} + \nabla \cdot \rho(\phi)\vec{U}\vec{U} - \nabla \cdot [2\mu(\phi)\mathbb{D} + \vec{U}\rho'(\phi)M(\phi)\nabla g_\phi] + \nabla p = -\phi\nabla g_\phi - \sum c_j \nabla g_{c_j}$
  - $\nabla \cdot \vec{U} = 0$
  - $\frac{\partial c_j}{\partial t} + \vec{U} \cdot \nabla c_j - \nabla \cdot \left(K_j(\phi) c_j \nabla g_{c_j}\right) = 0$
  - $\nabla \cdot (\epsilon_0 \epsilon \vec{E}) = \rho_e$
  - $[2\mu\mathbb{D} - p'\mathbb{I} + \gamma\kappa\mathbb{I} + \epsilon_0\epsilon\vec{E}\vec{E} - \frac{1}{2}\epsilon_0\epsilon E^2\mathbb{I}] \cdot \hat{n} = 0$
  - $\frac{\partial \phi}{\partial t} + \vec{U} \cdot \nabla\phi - \nabla \cdot (M(\phi)\nabla g_\phi) = 0$
- Chemical potential of species c_j and the phase field ϕ
  - $g_{c_j}(c_j, \phi) = \alpha'(c_j) + \beta_j(\phi) + z_j V$
  - For dilute solutions: $\alpha(c) = c(\log(c) - 1)$
  - $g_\phi = \frac{\partial f}{\partial \phi} - \nabla \cdot \frac{\partial f}{\partial \nabla\phi} + \sum \beta_j'(\phi) c_j - \frac{1}{2}\epsilon'(\phi)|\nabla V|^2$
  - $f(\phi, \nabla\phi) = \frac{3\sigma}{2\sqrt{2}}\left[\frac{\epsilon}{2}|\nabla\phi|^2 + \epsilon^{-1}W(\phi)\right]$
  - $W(\phi) = \frac{(1-\phi^2)^2}{4}$
- Phase field mobility: $M(\phi) = \epsilon M_0$ or $M(\phi) = M_0 * \max(1 - \phi^2)$

CLSVOF based simulations

Drop-Drop, Situation before contact

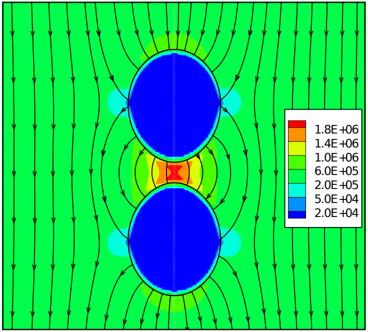


Figure: Efield before contact

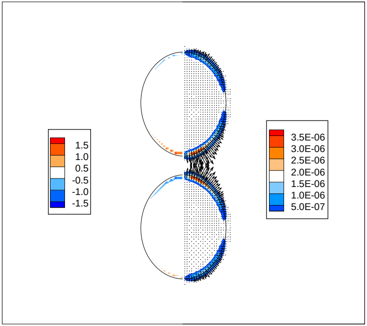


Figure: Charge & Eforce before contact

CLSVOF based simulations

Drop-Drop, Situation at contact

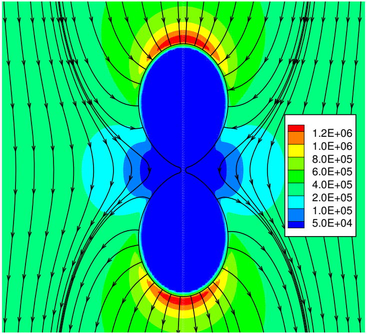


Figure: Efield at contact

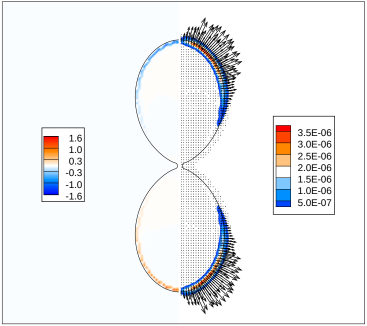


Figure: Charge & Eforce at contact

CLSVOF based simulations

Drop-Drop, Situation after contact

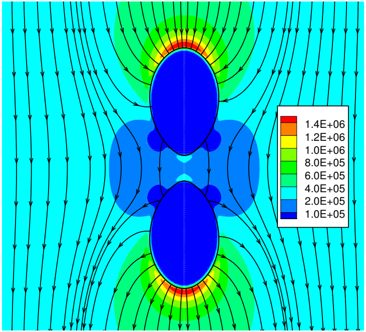


Figure: Efield after contact

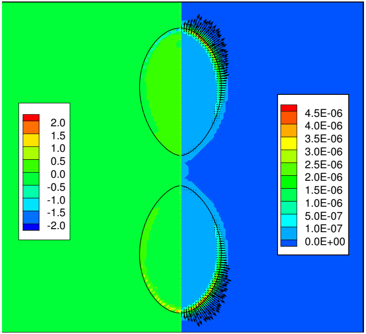


Figure: Charge & Eforce after contact

Drop-Interface Interactions

Situation before contact

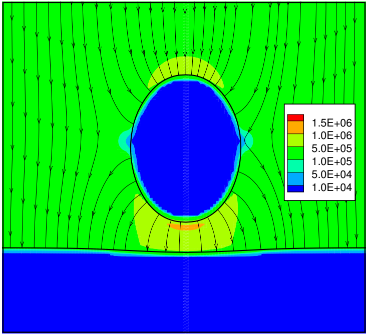


Figure: Efield before contact

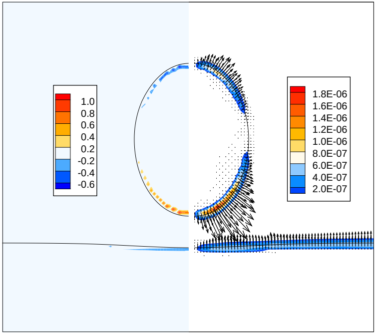


Figure: Charge & Eforce before contact

Drop-Interface Interactions

Situation at contact

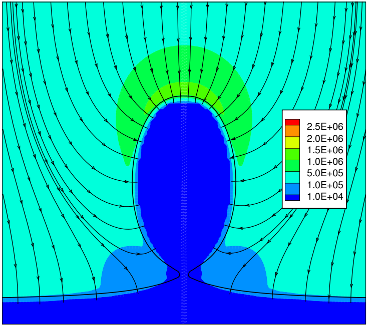


Figure: Efield at contact

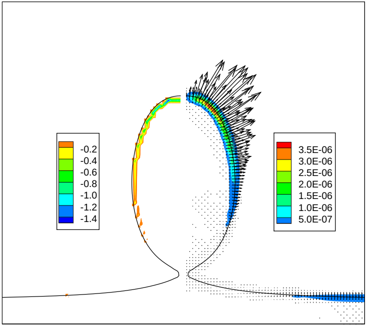


Figure: Charge & Eforce at contact

Drop-Interface Interactions

Situation after contact

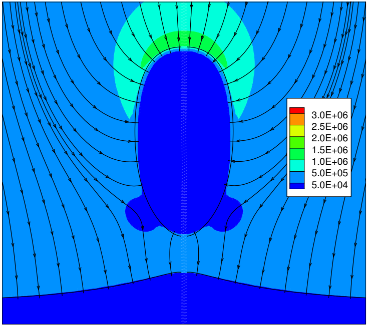


Figure: Efield after contact

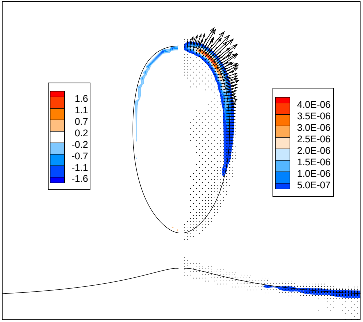


Figure: Charge & Eforce after contact

Drop-Interface Interactions

Drop-Interface, Greater velocity after contact

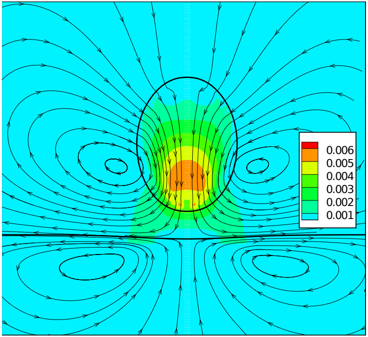


Figure: Velocity before contact

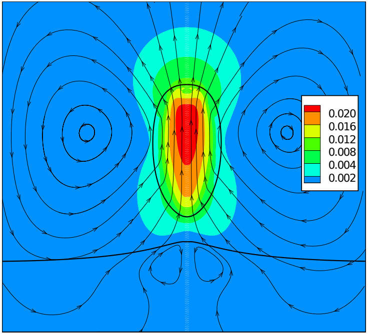
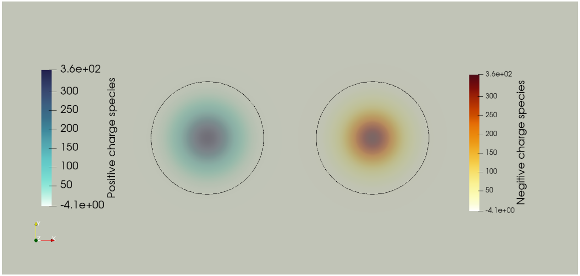


Figure: Velocity after contact

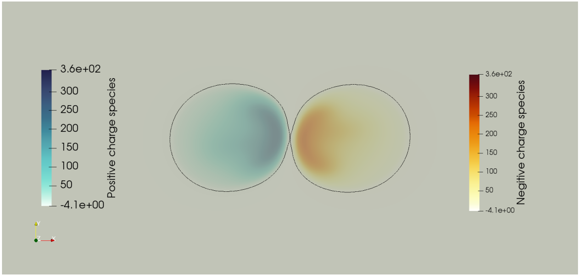
BERNAISE based results

Distribution of charged species

- Initial distribution



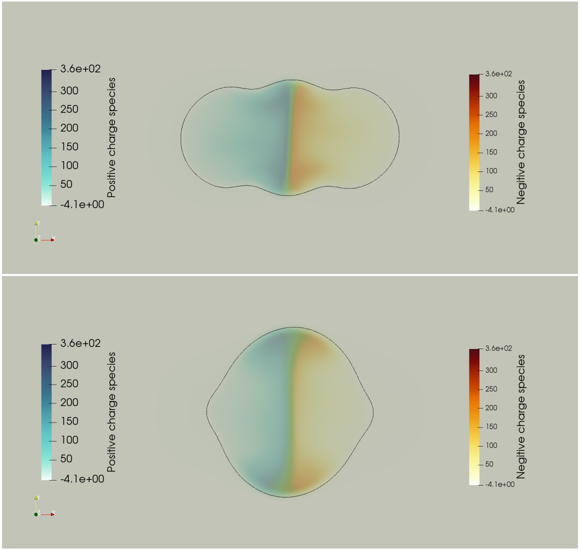
- Just before contact



BERNAISE based results

Distribution of charged species

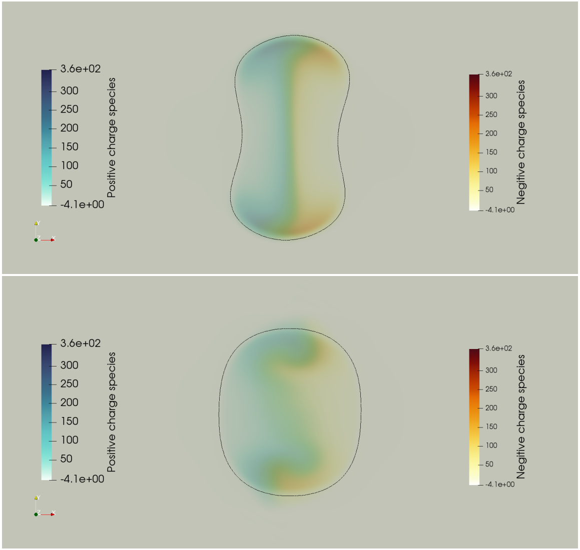
- During contact
- During contact



BERNAISE based results

Distribution of charged species

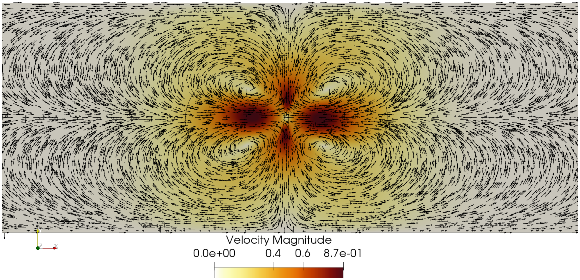
- During contact
- During contact



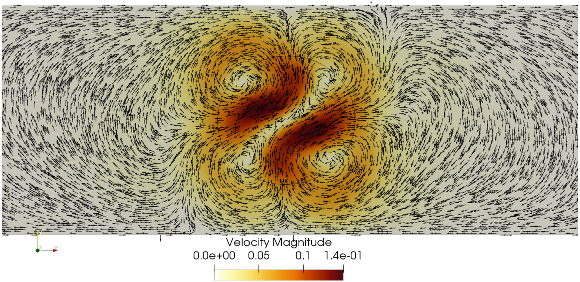
BERNAISE based results

Velocity distribution in the domain

- Before contact



- After contact



Thank you for your attention.
Questions...