Numerical simulations for a leaky dielectric drop under DC electric field

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A leaky dielectric droplet under DC electric field

Questions:
- How does the droplet respond?
- What is the circulatory flow pattern?

Applications: droplet manipulation in micro-fluidic system; mixing inside the droplet, inject printing etc.

Conductivity $\sigma$: a measure of a material’s ability to conduct an electric current.

Permittivity $\varepsilon$: or dielectric constant, a measure of how easily a dielectric material polarizes in response to an electric field;
Experiments vs. Simulations

Figure: Left: Experiments from Torza et al. 1971, Right: Present simulations
Experimental work


Small deformation theory

- G.I. Taylor (1966), creeping flow, small perturbation from sphericity, first order approximation, able to predict oblate or prolate shape; O. O. Ajaji (1978), second order approximation; J. Q. Feng (2002), 2D Electrorotation, first order result

Numerical simulations


Interfacial stresses balance

Along the interface, hydrodynamic stress + electric (Maxwell) stress + interfacial tension = 0;

\[ [T_V + M_E] \Sigma \cdot n + \gamma \kappa n = 0 \]

where \([\Phi]_\Sigma = \Phi^+ - \Phi^-\); \(n\) is the outward normal; \(\gamma\): interfacial tension; \(\kappa\): curvature

\[ T_V = -pI + \mu(\nabla u + \nabla u^T) \]

\[ M_E = \varepsilon(EE - \frac{1}{2}(E \cdot E)I) \]
Navier Stokes + capillary and electric effects

Interface representation: \( \Sigma = \{ \mathbf{X}(s, t) = (X(s, t), Y(s, t)) \} \)

\[
\rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{f}_C + \mathbf{f}_E \quad \text{in } \Omega
\]

\[\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega\]

\[
\frac{\partial \mathbf{X}}{\partial t}(s, t) = \mathbf{U}(s, t) = \int_{\Omega} \mathbf{u}(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) \, d\mathbf{x} \quad \text{on } \Sigma
\]

\[
f_C = \int_{\Sigma} \frac{\partial}{\partial s}(\gamma \mathbf{r}) \delta(\mathbf{x} - \mathbf{X}(s, t)) \, ds
\]

Question: what is the electric force \( \mathbf{f}_E \)?
Electric force field

Eulerian electric volume force

- Maxwell stress tensor $\mathbf{M}_E = \varepsilon \left( \mathbf{EE} - \frac{1}{2}(\mathbf{E} \cdot \mathbf{E})I \right)$
- $\mathbf{f}_E = \nabla \cdot \mathbf{M}_E = -\frac{1}{2}(\mathbf{E} \cdot \mathbf{E})\nabla \varepsilon + \nabla \cdot (\varepsilon \mathbf{E}) \mathbf{E}$
- Across the interface, $\mathbf{E} \cdot \mathbf{\tau}$ is continuous but $\mathbf{E} \cdot \mathbf{n}$ has a jump discontinuity
- Using smoothing numerical method, $\mathbf{E}$ has $O(1)$ error and $\mathbf{f}_E$ has $O(1/h)$ error near the interface

Lagrangian electric interfacial force

- $\mathbf{F}_E = [\mathbf{M}_E \cdot \mathbf{n}] = (\mathbf{M}_E^+ - \mathbf{M}_E^-) \cdot \mathbf{n}$; where $\mathbf{M}_E^\pm$: Maxwell stress tensor inside (−) and outside (+) of the drop
- Necessary to the Boundary Integral Method
- Compute $\mathbf{M}_E^\pm$ accurately
- Then $\mathbf{f}_E = \int_\Sigma \mathbf{F}_E(s, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) |\mathbf{X}_s| \, ds$
What is the explicit from of $\mathbf{F}_E$?

Let $\mathbf{J} = \sigma \mathbf{E}$ (current density) and express $\mathbf{E} = E_n \mathbf{n} + E_\tau \mathbf{\tau}$.

\[
\mathbf{M}_E \cdot \mathbf{n} = \varepsilon \left( \mathbf{EE} - \frac{1}{2}(\mathbf{E} \cdot \mathbf{E}) \mathbf{I} \right) \cdot \mathbf{n}
\]
\[
= \varepsilon E_n (E_n \mathbf{n} + E_\tau \mathbf{\tau}) - \frac{\varepsilon}{2} (E_n^2 + E_\tau^2) \mathbf{n}
\]
\[
= \frac{\varepsilon}{\sigma^2} (\sigma E_n)^2 \mathbf{n} + \frac{\varepsilon}{\sigma} (\sigma E_n) E_\tau \mathbf{\tau} - \frac{\varepsilon}{2\sigma^2} (\sigma E_n)^2 \mathbf{n} - \frac{\varepsilon}{2} E_\tau^2 \mathbf{n}
\]
\[
= \frac{\varepsilon}{2\sigma^2} (\sigma E_n)^2 \mathbf{n} + \frac{\varepsilon}{\sigma} (\sigma E_n) E_\tau \mathbf{\tau} - \frac{\varepsilon}{2} E_\tau^2 \mathbf{n}
\]
\[
= \frac{1}{2} \left( J_n^2 \frac{\varepsilon}{\sigma^2} - E_\tau^2 \varepsilon \right) \mathbf{n} + \frac{\varepsilon}{\sigma} J_n E_\tau \mathbf{\tau} \quad \text{where } J_n = \mathbf{J} \cdot \mathbf{n}.
\]

Note, $[E_\tau] = 0$ and $[J_n] = 0$ (no charge flux). Thus, the interfacial electric force can be written as

\[
\mathbf{F}_E = (\mathbf{M}^+_E - \mathbf{M}^-_E) \cdot \mathbf{n}
\]
\[
= \frac{1}{2} \left( J_n^2 \left( \frac{\varepsilon^+}{(\sigma^+)^2} - \frac{\varepsilon^-}{(\sigma^-)^2} \right) - E_\tau^2 (\varepsilon^+ - \varepsilon^-) \right) \mathbf{n} + J_n E_\tau \left( \frac{\varepsilon^+}{\sigma^+} - \frac{\varepsilon^-}{\sigma^-} \right) \mathbf{\tau}.
\]

Exactly same as the continuous electric surface force derived by Tomar et al. (2007)
How to compute the electric field \( \mathbf{E} \)?

- \( q_v = \nabla \cdot (\varepsilon \mathbf{E}) \): volume-charge density

- Charge conservation law is expressed as

\[
\frac{D}{Dt}q_v + \nabla \cdot (\sigma \mathbf{E}) = 0
\]

- **Leaky dielectric model** (G. I. Taylor 1966):
  \( t_E = \varepsilon / \sigma \ll t_f = \rho L^2 / \mu \); the charge accumulates at the interface almost instantaneously as compared to the fluid motion, thus the charge density equation can be simplified as

\[
\nabla \cdot (\sigma \mathbf{E}) = 0
\]

- Absence of time-varying magnetic field and Maxwell-Faraday equation \( \Rightarrow \nabla \times \mathbf{E} = 0 \Rightarrow \mathbf{E} = -\nabla \phi \)

- Electric potential and electric charge flux are both continuous across the interface

\[
\nabla \cdot (\sigma \nabla \phi) = 0 \quad \text{in} \ \Omega, \quad [\phi] = 0 \quad \text{and} \quad [\sigma \phi_n] = 0 \quad \text{on} \ \Sigma
\]
Potential equation for lipid bilayer membrane in vesicle electrohydrodynamics

\[
\Delta \phi = 0 \quad \text{in } \Omega \setminus \Sigma
\]

\[
[\phi] = V_m \quad \text{and} \quad [\sigma \nabla \phi \cdot \mathbf{n}] = 0 \quad \text{on } \Sigma
\]

\[
C_m \frac{dV_m}{dt} + G_m V_m = \sigma^+ \nabla \phi^+ \cdot \mathbf{n} = \sigma^- \nabla \phi^- \cdot \mathbf{n}, \quad \text{on } \Sigma
\]

where \(C_m\) and \(G_m\) are effective capacitance and conductance, respectively.
A simple immersed interface method for solving elliptic problems with interfaces

- A piecewise coefficient elliptic interface problem

\[ \nabla \cdot (\sigma \nabla \phi) = f \quad \text{in } \Omega \setminus \Sigma, \quad [\phi] = v(s), \quad [\sigma \phi_n] = w(s) \quad \text{on } \Sigma \]

- Introduce an interface augmented variable \( g \) such that

\[
\Delta \phi = \begin{cases} 
  \frac{f^-}{\sigma^-} & \text{in } \Omega^- \\
  \frac{f^+}{\sigma^+} & \text{in } \Omega^+ 
\end{cases} \quad [\phi] = v(s), \quad [\phi_n] = g(s), \quad [\sigma \phi_n] = w(s)
\]

- One of the following two derived identities for \([\phi_n]\) must be imposed

\[
\phi_n^+ + \frac{\sigma^-}{[\sigma]} [\phi_n] = \frac{[\sigma \phi_n]}{[\sigma]}, \quad \text{if } \sigma^- > \sigma^+ \\
\phi_n^- + \frac{\sigma^+}{[\sigma]} [\phi_n] = \frac{[\sigma \phi_n]}{[\sigma]}, \quad \text{if } \sigma^+ > \sigma^-
\]

Regular and irregular points for 5-point Laplacian

\[
\Sigma = \sum_{x_{i,j}} c_{x_{i,j}} - 1 \quad c_{x_{i-1,j}} c_{x_{i,j}} + 1 c_{S} \quad X^\ast \quad \Omega^+ \\
X^\times \quad \Omega^- \\
x_{i-1,j} \quad x_{i,j} \quad x_{i+1,j} \\
\Sigma \\
x_{i,j-1} 
\]
A simple IIM to incorporate the normal jumps, Russel & Wang (2003)

\[
\Delta_h \phi = \frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}}{h^2} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{h^2}
\]

\[
= \frac{\phi_{i-1,j}^+ - 2\phi_{i,j}^- + \phi_{i+1,j}^-}{h^2} + \frac{\phi_{i,j+1}^+ - 2\phi_{i,j}^- + \phi_{i,j-1}^-}{h^2}
\]

\[
+ \frac{\phi_{i-1,j}^- - \phi_{i-1,j}^-}{h^2} + \frac{\phi_{i,j+1}^- - \phi_{i,j+1}^-}{h^2}
\]

\[
= (\phi_{xx}^-)_{i,j} + (\phi_{yy}^-)_{i,j} + O(h^2) + \frac{\phi_{i-1,j}^c}{h^2} + \frac{\phi_{i,j+1}^c}{h^2}
\]

\[
= f_{i,j}^- + \frac{1}{h^2} (\phi_{i-1,j}^c + \phi_{i,j+1}^c) + O(h^2).
\]
\[
\phi_{i-1,j} = \phi_{i-1,j}^+ - \phi_{i-1,j}^-
\]

\[
= \left( \phi^*_+ + d \frac{\partial \phi^*_+}{\partial n} + \frac{d^2}{2} \frac{\partial^2 \phi^*_+}{\partial n^2} + O(h^3) \right) \\
- \left( \phi^*_- + d \frac{\partial \phi^*_-}{\partial n} + \frac{d^2}{2} \frac{\partial^2 \phi^*_-}{\partial n^2} + O(h^3) \right)
\]

\[
= [\phi]_{x^*} + d \left[ \frac{\partial \phi}{\partial n} \right]_{x^*} + \frac{d^2}{2} \left[ \frac{\partial^2 \phi}{\partial n^2} \right]_{x^*} + O(h^3).
\]

\[\blacktriangleright\] \(d\) is the signed distance between the grid point \(x_{i-1,j}\) and the projection \(X^*\).
On the interface, we use the equation

\[
\frac{\partial^2 \phi}{\partial n^2} + \kappa \frac{\partial \phi}{\partial n} + \nabla_s^2 \phi = f
\]

where \(\kappa\) is the local curvature of the interface. Then,

\[
\left[\frac{\partial^2 \phi}{\partial n^2}\right]_{X^*} = [f]_{X^*} - \kappa_{X^*} \left[\frac{\partial \phi}{\partial n}\right]_{X^*} - \nabla_s^2 [\phi]_{X^*}.
\]

Thus, the final correction term can be obtained as

\[
\phi_{i-1,j}^{c} = [\phi]_{X^*} + d \left[\frac{\partial \phi}{\partial n}\right]_{X^*} + \frac{d^2}{2} \left[\frac{\partial^2 \phi}{\partial n^2}\right]_{X^*}
\]

\[
= [\phi]_{X^*} + d \left[\frac{\partial \phi}{\partial n}\right]_{X^*} + \frac{d^2}{2} \left( [f]_{X^*} - \kappa_{X^*} \left[\frac{\partial \phi}{\partial n}\right]_{X^*} - \nabla_s^2 [\phi]_{X^*} \right).
\]

The correction term \(\phi_{i,j+1}^{c}\) can be computed similarly.
The discretized equation by finite difference method can be written as

$$\Delta_h \phi_{ij} + \frac{\phi_{ij}^c}{h^2} = f_{ij}$$

Here $\phi_{ij}^c = 0$ at regular points, and at irregular points,

$$\phi_{ij}^c = [\phi]x^* + d[\phi_n]x^* + \frac{d^2}{2} \left([f]x^* - \kappa x^*[\phi_n]x^* - \nabla_s^2[\phi]x^*\right)$$

Reference: Russel & Wang (2003), Poisson equation; Lai & Tseng (2008), Stokes equations; Xu (2012), piecewise coefficient Poisson equation
Compute one-sided normal derivative along the interface by least square approximation

\[ \Omega^{-} \rightarrow \Omega^{+} \]

Assume \( \sigma^{-} > \sigma^{+} \)

- \( \phi_{n}^{+} + \frac{\sigma^{-}}{[\sigma]}[\phi_{n}] = \frac{[\sigma \phi_{n}]}{[\sigma]} \)
- At each orthogonal projection \( X^{*} \), we use blue nodes to construct least squares polynomial \( P(x, y) \Rightarrow \min \sum_{i,j} (P_{i,j} - \phi_{i,j})^2 \)
- Approximate \( \phi_{n}^{+}(X^{*}) \approx \nabla P(X^{*}) \cdot n(X^{*}) = B^{+} \phi \)
- \( B^{+} \phi + \frac{\sigma^{-}}{[\sigma]}[\phi_{n}] = \frac{[\sigma \phi_{n}]}{[\sigma]} \)
Compute one-sided normal derivative along the interface by normal extrapolation, Xu (2012)

\[ \phi^+_n(\mathbf{X}^*_k) = \frac{-5\phi(S_1) + 8\phi(S_2) - 3\phi(S_3)}{2\overline{h}} + O(\overline{h}^2), \]

- Approximate \( \phi^+_n(\mathbf{X}^*_k) = B^+\phi \) by above extrapolating formula, where \( \overline{h} = (1 + \epsilon)\sqrt{2} \)

\( h \) with a small regularization parameter \( \epsilon = 10^{-10} \)

- \( B^+\phi + \frac{\sigma^-}{[\sigma]}[\phi_n] = \frac{[\sigma\phi_n]}{[\sigma]} \)
Let \( \Phi \) and \( \Psi \) be the solution vectors formed by \( \phi_{ij} \) and \([\phi_n]x^*\). The resultant matrix equation becomes

\[
\begin{bmatrix}
\Delta_h & E \\
B^+ & \frac{\sigma^-}{[\sigma]} I \\
\end{bmatrix} \begin{bmatrix}
\Phi \\
\Psi \\
\end{bmatrix} = \begin{bmatrix}
F \\
G \\
\end{bmatrix}
\]

**Step 1.** Solve a Poisson equation for intermediate solution \( \Phi^* \) by

\[
\Delta_h \Phi^* = F
\]

This can be solved efficiently by one fast Poisson solver.

**Step 2.** Solve \( \Psi \) by

\[
\left( B^+ \Delta_h^{-1} E - \frac{\sigma^-}{[\sigma]} I \right) \Psi = B^+ \Phi^* - G
\]

This linear system is solved by GMRES iterative method with a stopping criteria chosen as \( O(h^2) \).

**Step 3.** After solving \( \Psi \), we then solve \( \Phi \) by

\[
\Delta_h \Phi = F - E \Psi.
\]

Again, this involves applying one fast Poisson solver.
Question: We obtain $\phi$ on the grid and $[\phi_n]$ on those projection points, how can we compute $\nabla \phi$?

- $\phi$ is computed at the cell center, so that $\phi_x$ and $\phi_y$ are computed at right and top edges, respectively;
- For instance, $\phi_x(x_{i-1/2,j})$, where $x_{i-1/2,j} = x^-$ locates on $\Omega^-$ side

\[
\frac{\phi^+_i,j - \phi^-_{i-1,j}}{h} = \frac{\phi^-_{i,j} - \phi^-_{i-1,j} + \phi^+_i,j - \phi^-_{i,j}}{h} = \phi_x(x^-) + O(h^2) + \frac{\phi^+_i,j - \phi^-_{i,j}}{h}
\]

Therefore,

\[
\phi_x(x^-) \approx \frac{\phi^+_i,j - \phi^-_{i-1,j}}{h} - \frac{\phi^-_i,j}{h}
\]

- $\phi_y$ can be approximated similarly
Example 1: Convergence and efficiency test

- Exact solution $\phi(x, y)$ in $\Omega = [-1, 1] \times [-1, 1]$ defined by
  \[
  \phi(x, y) = \begin{cases} 
  \exp(x + y) & x \in \Omega^-, \\
  \sin x \sin y & x \in \Omega^+.
  \end{cases}
  \]

- Interface $\Sigma = \{(\frac{x}{a})^2 + (\frac{y}{b})^2 = 1\}$ with $a = 0.2$ and $b = 0.5$

\[
\sigma_r = 10
\]

| $M$ | $||\phi_h - \phi_e||_\infty$ rate | $||(\phi_h)_x - (\phi_e)_x||_\infty$ rate | $||(\phi_h)_y - (\phi_e)_y||_\infty$ rate | iter |
|-----|----------------------------------|----------------------------------|----------------------------------|------|
| 32  | 3.31E-04                         |        2.51E-03                  | 1.75E-03                         | 7    |
| 64  | 8.46E-05                         | 1.97   3.42E-04                  | 3.84E-04                         | 9    |
| 128 | 2.43E-05                         | 1.80   9.85E-05                  | 1.13E-04                         | 10   |
| 256 | 5.37E-06                         | 2.18   3.84E-05                  | 3.50E-05                         | 10   |

\[
\sigma_r = 0.1
\]

| $M$ | $||\phi_h - \phi_e||_\infty$ rate | $||(\phi_h)_x - (\phi_e)_x||_\infty$ rate | $||(\phi_h)_y - (\phi_e)_y||_\infty$ rate | iter |
|-----|----------------------------------|----------------------------------|----------------------------------|------|
| 32  | 7.99E-04                         |        5.07E-03                  | 5.16E-03                         | 6    |
| 64  | 1.27E-04                         | 2.65   5.21E-04                  | 6.10E-04                         | 3.08  |
| 128 | 3.08E-05                         | 2.04   1.91E-04                  | 2.52E-04                         | 1.28  |
| 256 | 5.37E-06                         | 2.52   2.85E-05                  | 3.12E-05                         | 3.01  |
Example 2: Comparison with smoothing method

- Smoothing method:
  - Solve the indicator function $H(x)$ by
    \[
    \Delta H(x) = -\nabla \cdot \int_{\Sigma} n\delta(x - X(s))|X_s| \, ds
    \]
  - Smooth $\sigma$ through harmonic mean average as
    \[
    \frac{1}{\sigma(x)} = \frac{H(x)}{\sigma^-} + \frac{1 - H(x)}{\sigma^+}
    \]

- Exact solution $\phi(x, y)$ in $\Omega = [-1, 1] \times [-1, 1]$ defined by
  \[
  \phi(x, y) = \begin{cases}
  a_2(x^2 + y^2) + a_1 & x \in \Omega^-, \\
  (x^2 + y^2)^{1.5} & x \in \Omega^+.
  \end{cases}
  \]

- Interface $\Sigma = \{(\frac{x}{a})^2 + (\frac{y}{b})^2 = 1\}$ with $a = 0.5$ and $b = 0.5$

- $\sigma_r = 0.1$, chose $a_1$ and $a_2$ to satisfy $[\phi] = 0$ and $[\sigma \phi_n] = 0$

<table>
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<th>$M$</th>
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<th>$|\phi_{hS} - \phi_e|_\infty$</th>
<th>$|(\phi_h)x - (\phi_e)x|_\infty$</th>
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</table>
Nondimensionalization

Dimensionless variables

\[ x^* = \frac{x}{R}, \quad t^* = \sqrt{\frac{\gamma_\infty}{\rho R^3}} t, \quad u^* = \sqrt{\frac{\rho R}{\gamma_\infty}} u, \quad p^* = \frac{R}{\gamma_\infty} p, \]

\[ \varepsilon^* = \frac{\varepsilon}{\varepsilon^+}, \quad \sigma^* = \frac{\sigma}{\sigma^+}, \quad E^* = \frac{E}{E_\infty}. \]

Here \( R \) is the initial drop radius. We define the ratio

\[ \sigma_r = \frac{\sigma^-}{\sigma^+}, \quad \varepsilon_r = \frac{\varepsilon^-}{\varepsilon^+}. \]
Dimensionless governing equations

- Navier-Stokes equations:

\[
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + Oh \Delta \mathbf{u} + \int_{\Sigma} (\mathbf{F}_C + Ca_E \mathbf{F}_E |\mathbf{X}_s|) \delta(\mathbf{x} - \mathbf{X}) \, ds
\]

\[
\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega
\]

\[
\mathbf{F}_C = \frac{\partial}{\partial s}(\gamma \tau) \quad \text{on } \Sigma
\]

\[
\nabla \cdot (\sigma \nabla \phi) = 0 \quad \text{in } \Omega, \quad [\phi] = 0, \quad [\sigma \phi_n] = 0
\]

\[
\mathbf{E} = -\nabla \phi, \quad \mathbf{M}_E = \varepsilon \left(\mathbf{E} \mathbf{E} - \frac{1}{2} (\mathbf{E} \cdot \mathbf{E}) \mathbf{I}\right), \quad \mathbf{F}_E = (\mathbf{M}_E^+ - \mathbf{M}_E^-) \cdot \mathbf{n}
\]

\[
\frac{\partial \mathbf{x}}{\partial t}(s, t) = \mathbf{U}(s, t) = \int_{\Omega} \mathbf{u}(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) \, d\mathbf{x} \quad \text{on } \Sigma
\]

Ohnesorge number: \( Oh = \mu / \sqrt{\gamma_\infty \rho R} \)

Electric capillary number: \( Ca_E = \varepsilon^+ R E_\infty^2 / \gamma_\infty \)
Given $\mathbf{u}^n, \mathbf{X}^n$, need to advance one time step to find $\mathbf{u}^{n+1}, \mathbf{X}^{n+1}$

1. Compute the electric potential $\phi^n$ by the developed augmented IIM. Use the values of $\phi^n$ to compute the electric field $\mathbf{E}^n = (-\phi^n_x, -\phi^n_y)$ and then we perform one-sided interpolation to compute the Maxwell stresses $\mathbf{M}^+_E$ and $\mathbf{M}^-_E$ to obtain the interfacial electric force $\mathbf{F}^n_E$ at Lagrangian interface markers.

2. Compute the interfacial tension force $\mathbf{F}^n_C$.

3. Distribute the interfacial tension $\mathbf{F}^n_C$ and electric force $\mathbf{F}^n_E$ from the Lagrangian markers into the fluid grid points by using the discrete delta function.

4. Solve the Navier-Stokes equations by the projection method to obtain new velocity $\mathbf{u}^{n+1}$.

5. Interpolate the new velocity on the fluid grid point to the marker points, and then move the marker points to new positions $\mathbf{X}^{n+1}$.
Dynamic control of markers distribution, Lai, Tseng & Huang CiCP 2010

Goal: To make the surface markers to be equidistributed in arc-length along the interface without changing the shape of the interface (Hou, Lowengrub and Shelley; arclength-tangent angle formulation 1994)

Idea: To introduce an artificial tangential velocity such that the marker $X(s, t)$ satisfies $|X_s|_s = 0$.

\[
\frac{\partial X(s, t)}{\partial t} = U(s, t) + U^A(s, t) \tau = \int_\Omega u(x, t) \delta(x - X(s, t)) dx + U^A(s, t) \tau
\]

Let $L_s = \left| \frac{\partial X}{\partial s} \right| = |X_s|$. Then $|X_s|_s = L_s, s = 0$ implies that $L_s$ is independent of $s$ and is dependent on $t$.

\[
L_s(t) = \frac{1}{2\pi} \int_0^{2\pi} L_s'(s', t) \, ds'
\]

\[
L_{s, t}(t) = \frac{1}{2\pi} \int_0^{2\pi} L_{s', t}(s', t) \, ds'
\]
\[ L_{s,t} = \frac{\partial}{\partial t} |X_s| = \frac{\partial U}{\partial s} \cdot \tau + \frac{\partial U^A}{\partial s} \]

Proof:

\[
\frac{\partial}{\partial t} |X_s| = \frac{X_s \cdot X_{s,t}}{|X_s|} = \frac{X_s \cdot (U + U^A \tau)_s}{|X_s|} = \frac{1}{|X_s|} \left( X_s \cdot \left( \frac{\partial U}{\partial s} + \frac{\partial U^A}{\partial s} \tau + U^A \frac{\partial \tau}{\partial s} \right) \right) = \frac{\partial U}{\partial s} \cdot \tau + \frac{\partial U^A}{\partial s} = (\nabla_s \cdot U) |X_s| + \frac{\partial U^A}{\partial s} \]

\[
\left( \tau = \frac{X_s}{|X_s|}, \quad \frac{\partial \tau}{\partial s} = \kappa n |X_s|, \quad \nabla_s \cdot U = \frac{\partial U}{\partial \tau} \cdot \tau \right)
\]
Thus, we have

\[
\frac{\partial U}{\partial s} \cdot \tau + \frac{\partial U^A}{\partial s}(s, t) = \frac{1}{2\pi} \int_0^{2\pi} \frac{\partial U}{\partial s'} \cdot \tau' + \frac{\partial U^A}{\partial s'} ds'
\]

\[
= \frac{1}{2\pi} \int_0^{2\pi} \frac{\partial U}{\partial s'} \cdot \tau' ds'
\]

Integrating with respect to \( s \), we obtain

\[
U^A(s, t) - U^A(0, t) = \int_0^s \frac{\partial U}{\partial s'} \cdot \tau' ds' + \frac{s}{2\pi} \int_0^{2\pi} \frac{\partial U}{\partial s'} \cdot \tau' ds'
\]

Let \( U^A(0, t) = 0 \), we obtain the artificial tangential velocity as

\[
U^A(s, t) = \frac{s}{2\pi} \int_0^{2\pi} \frac{\partial U}{\partial s'} \cdot \tau' ds' - \int_0^s \frac{\partial U}{\partial s'} \cdot \tau' ds'
\]
Numerical results

Parameter setting

- $\Omega = [-4, 4] \times [-4, 4]$, Ohnesorge number $Oh = 1$, surface tension $\gamma = 1$
- Unless otherwise stated, we all use electric capillary number $Ca_E = 0.5$
- mesh width $h = 8/N$, marker spacing $\Delta s = 2\pi/M \approx h/2$
- Time step $\Delta t = h/4$ and initial drop radius $R = 1$

Numerical tests

1. Convergence test on interfacial electric force $F_E$
2. Convergence test on the fluid variables
3. Comparison with small-deformation theory
4. A leaky dielectric drop under shear flow
5. Large deformation for drop dynamics
Convergence test on interfacial electric force $F_E$

- $\sigma_r = 3$ and $\varepsilon_r = 2$
- For different grid size $M = 64, 128, 256, 512$ are chosen at $T = 2$
- Second-order convergence is obtained
Figure: The successive errors of the electric interfacial force $F_E$ in both $x$ and $y$ directions (see legends). The rate of convergence is around second-order.
Convergence test for the fluid variables

- $\sigma_r = 3$ and $\varepsilon_r = 2$
- Terminal time $T = 2$
- Successive error: $\|u_{2N} - u_N\|$ and rate $= \log_2 \frac{\|u_N - u_{N/2}\|}{\|u_{2N} - u_N\|}$

<table>
<thead>
<tr>
<th>$N$</th>
<th>$|u_{2N} - u_N|_\infty$</th>
<th>rate</th>
<th>$|v_{2N} - v_N|_\infty$</th>
<th>rate</th>
<th>$|X_{2N} - X_N|_\infty$</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>64</td>
<td>1.19E−02</td>
<td>-</td>
<td>1.62E−02</td>
<td>-</td>
<td>3.01E−02</td>
<td>-</td>
</tr>
<tr>
<td>128</td>
<td>2.84E−03</td>
<td>2.07</td>
<td>5.36E−03</td>
<td>1.60</td>
<td>8.80E−03</td>
<td>1.7</td>
</tr>
<tr>
<td>256</td>
<td>7.77E−04</td>
<td>1.87</td>
<td>8.85E−04</td>
<td>2.60</td>
<td>1.41E−03</td>
<td>2.6</td>
</tr>
</tbody>
</table>

Table: The mesh refinement results for the velocity components $u$ and $v$, the interface configuration $X$, and the relative volume loss of the drop at $T = 2$. 
Comparison with small-deformation theory

- Deformation factor \( D = \frac{L - B}{L + B} \), where \( L \) and \( B \) are drop extensions along the major and minor axes, respectively.

- Theoretical result: \( D = \frac{f_d(\sigma_r, \varepsilon_r)}{3(1+\sigma_r)^2} CaE \), where \( f_d \) is a discriminating function defined by \( f_d(\sigma_r, \varepsilon_r) = \sigma_r^2 + \sigma_r + 1 - 3\varepsilon_r \) (Feng, Journal of Colloid and Interface Science, 246 (2002), 112-121).

Figure: Solid line: \( \sigma_r = \varepsilon_r \); dash line: \( f_d = 0 \). “△”: Oblate and clockwise; “□”: prolate and clockwise; “○”: prolate and counterclockwise.
Three different flow behaviors
Physical explanations for drop shapes

- Charge relaxation time $t_E = \frac{\varepsilon}{\sigma}$: how fast conduction supplies charge to restore equilibrium

- $t^-_E = \frac{\varepsilon^-}{\sigma}$ and $t^+_E = \frac{\varepsilon^+}{\sigma}$

Case 1. oblate shape:
$t^-_E > t^+_E$
$\iff \frac{\varepsilon^-}{\sigma} > \frac{\varepsilon^+}{\sigma}$
$\iff \frac{\sigma^-}{\sigma} < \frac{\varepsilon^-}{\varepsilon^+}$
$\iff \sigma_r < \varepsilon_r$

Case 2. prolate shape:
$t^-_E < t^+_E$
$\iff \frac{\varepsilon^-}{\sigma} < \frac{\varepsilon^+}{\sigma}$
$\iff \frac{\sigma^-}{\sigma} > \frac{\varepsilon^-}{\varepsilon^+}$
$\iff \sigma_r > \varepsilon_r$
Figure: Equilibrium state of electric field $\mathbf{E}$ (left) and volume charge density $q_v$ (right).
A leaky dielectric drop under shear flow

Figure: The snapshots for a drop under shear flow $\mathbf{u} = (0.3y, 0)$ with (solid line) and without (dashed line) the electric effect. Top row: Case A; Middle row: Case B; Bottom row: Case C. $Ca_E = 1.0$. 

Large deformation for drop dynamics

Figure: The snapshots of drop dynamics with $\sigma_r = 10$ and $Ca_E = 1.5$. Top row: $\varepsilon_r = 1.37$; Bottom row: $\varepsilon_r = 0.5$. 
Conclusions

In this talk...

- We have developed a hybrid immersed boundary (IB) and immersed interface method (IIM) to simulate the dynamics of a leaky dielectric drop in Navier-Stokes flows.
- The electric potential is solved numerically by an augmented immersed interface method.
- Instead of applying the volume electric force, we alternatively treat the electric effect as an interfacial force bearing the normal jump of Maxwell stress on the interface.
- We put the capillary and electric forces in an unified immersed boundary formulation.
- Numerical results show good agreements with the theoretical and other numerical results.