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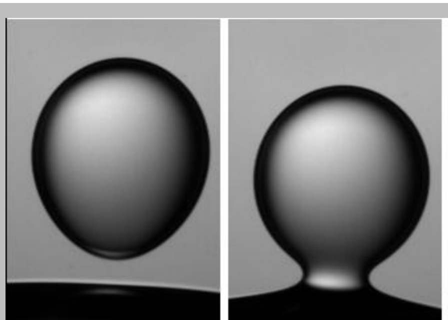

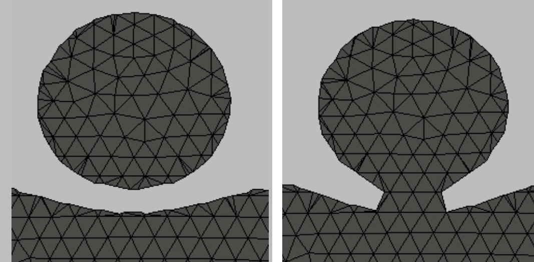

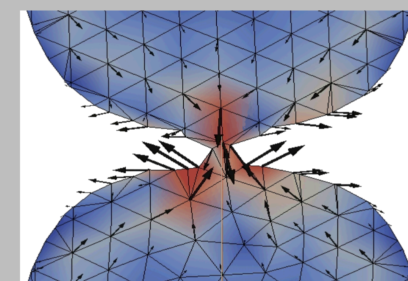

Interface-tracking hydrodynamic model for droplet electro-coalescence

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Experimental inspiration

- Many fluid-based technologies rely on electric fields to control droplet motion, e.g. high-speed droplet sorting for chemical reactions or purifying biodiesel fuel
- Ristenpart *et al*. *Nature* (2009) discovered that oppositely charged droplets can bounce rather than coalesce when the electric field is increased past a threshold

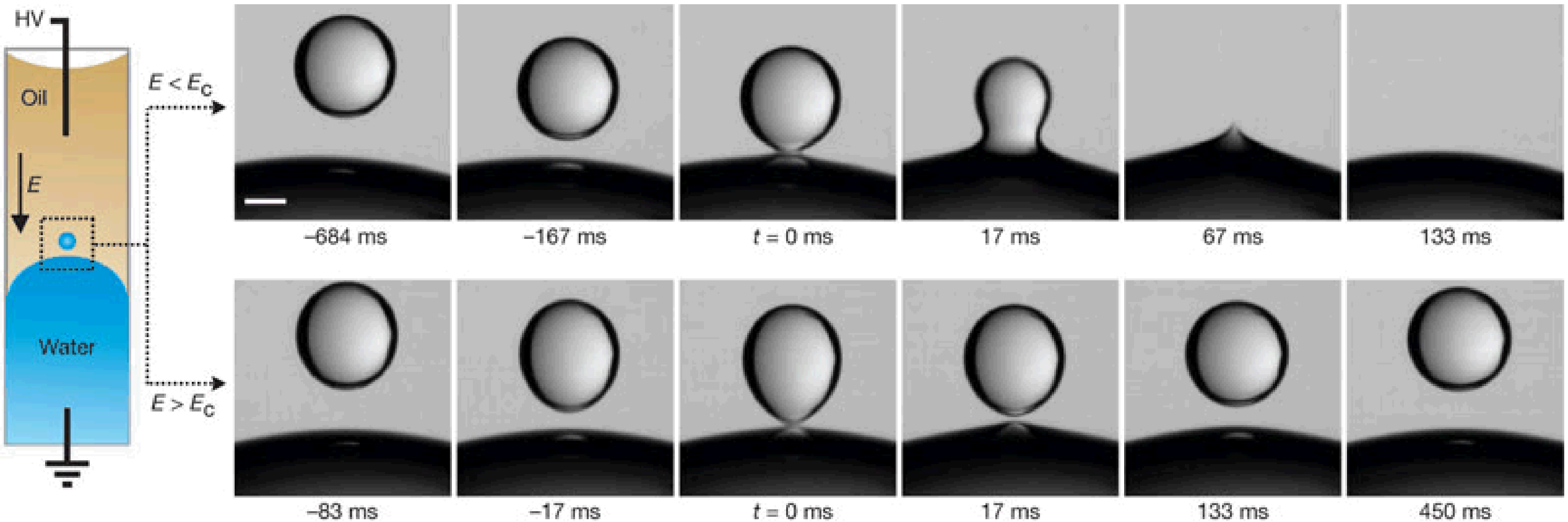
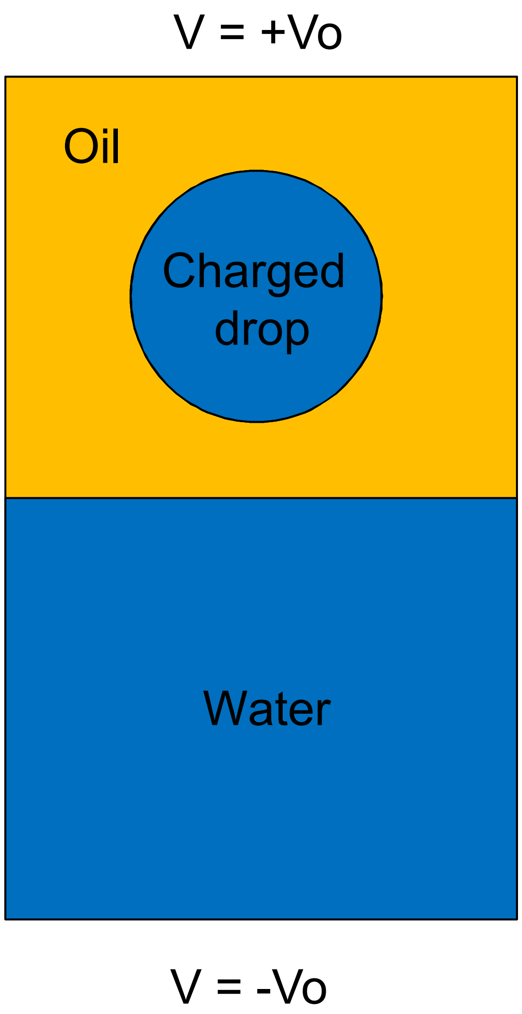


Figure courtesy of W. Ristenpart

Governing equations



- Fluid and material properties vary between two immiscible phases: density ρ, viscosity μ, permittivity ε, conductivity σ
- Incompressible Navier-Stokes with electric force:

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = -\nabla p + \nabla \cdot \left(\mu \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)\right) + \boldsymbol{F}_M$$

- Force due to electric field (divergence of the Maxwell stress tensor):

$$\boldsymbol{F}_M = \nabla \cdot \left(\varepsilon \left(\boldsymbol{E}\boldsymbol{E}^T - \frac{1}{2}(\boldsymbol{E} \cdot \boldsymbol{E})\mathbf{I}\right)\right) = \rho_V \boldsymbol{E} - \frac{1}{2}(\boldsymbol{E} \cdot \boldsymbol{E})\nabla \varepsilon$$

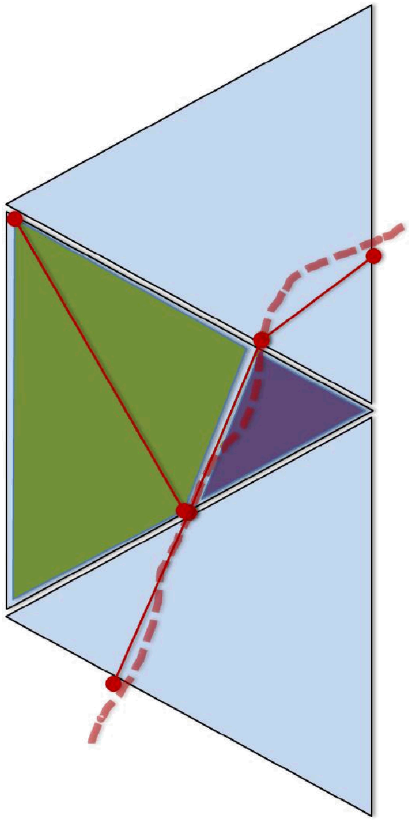
- Charge density and voltage equations:

$$\frac{\partial \rho_V}{\partial t} + \nabla \cdot (\sigma \boldsymbol{E} + \rho_V \boldsymbol{u}) = 0$$

$$\nabla \cdot (\varepsilon \boldsymbol{E}) = \rho_V$$

CDFEM: an interface-tracking method

- Conformal decomposition finite element method (CDFEM)



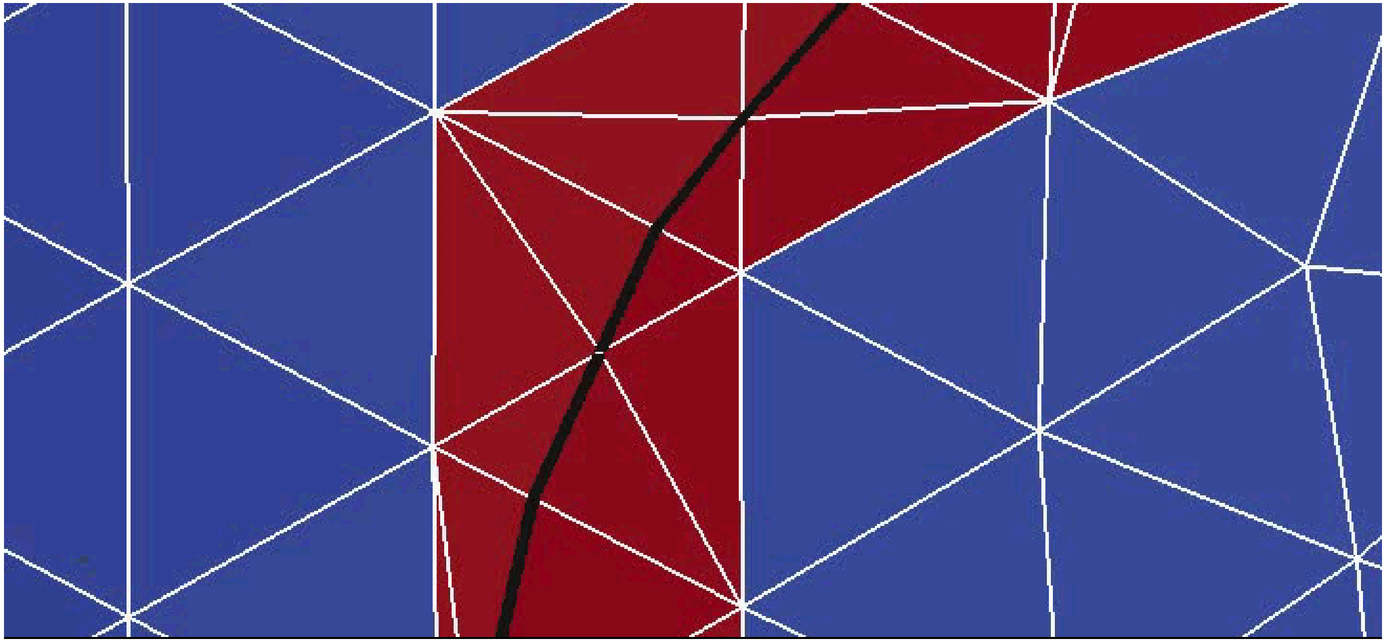
- A level set equation is used to track the interface

$$\frac{\partial \varphi}{\partial t} + \boldsymbol{u} \cdot \nabla \varphi = 0$$

- Interfacial properties, such as surface tension ($\gamma\kappa\mathbf{n}$) are computed at the interface and applied as boundary conditions instead of smeared Dirac delta functions in the bulk equations

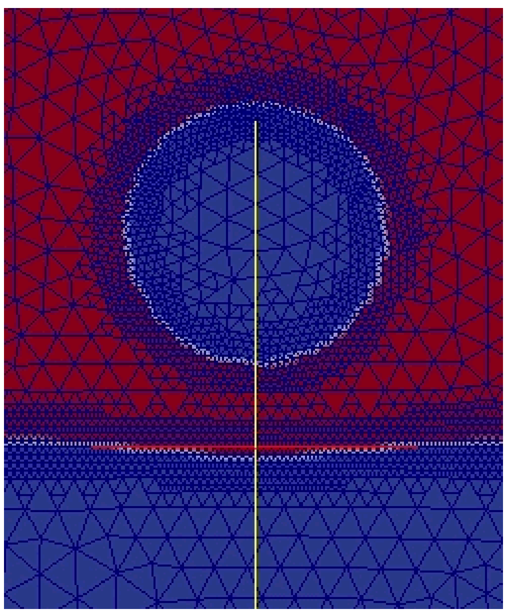
CDFEM: an interface-tracking method

- Sharp interface method that dynamically cuts elements at interface (tri/tet)

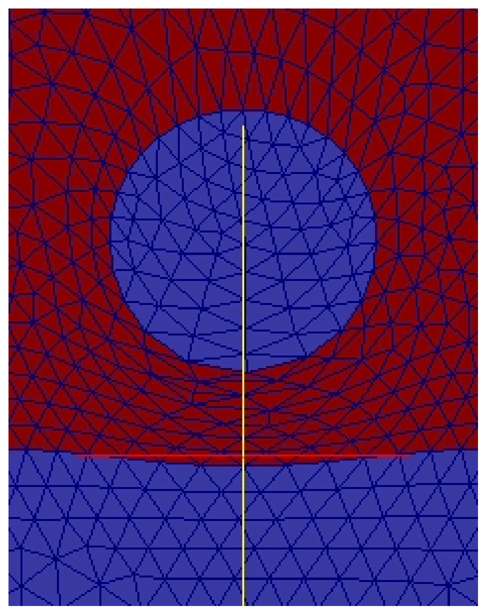


Interface method comparison

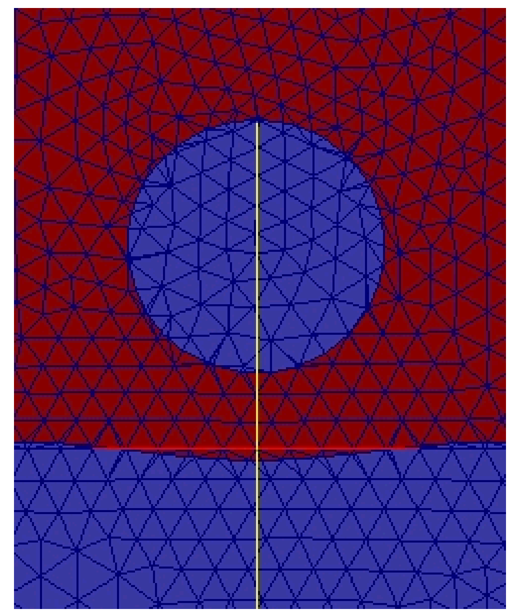
- Diffuse level set – interface gets smeared
- ALE (Arbitrary Lagrangian Eulerian) – elements need to be deleted/added as droplet merges (but can define shell elements)
- CDFEM – minimal new elements created (a tri/tet mesh necessary for decomposition algorithm)



Diffuse level set



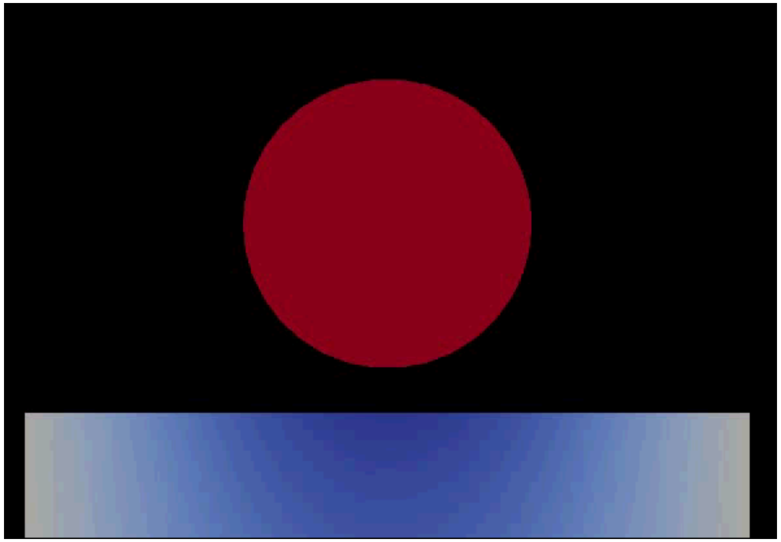
ALE

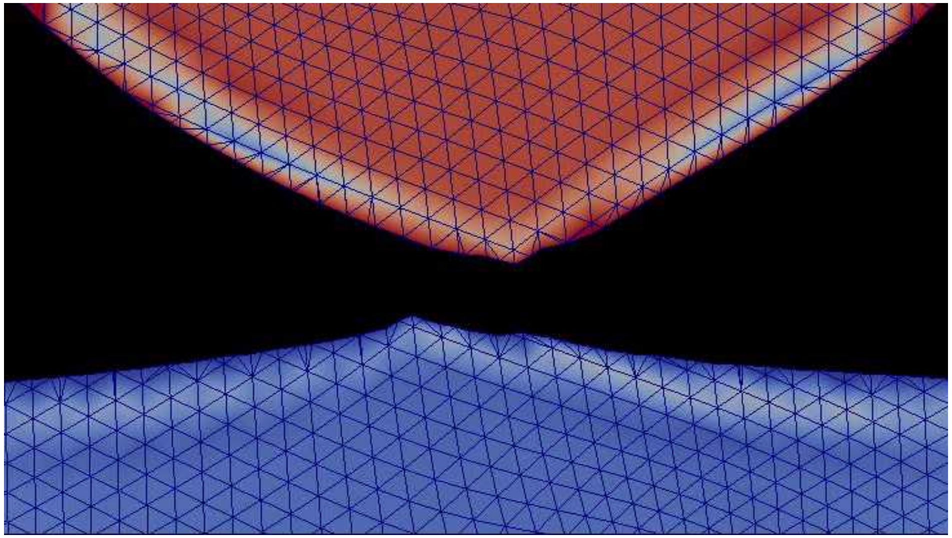


CDFEM

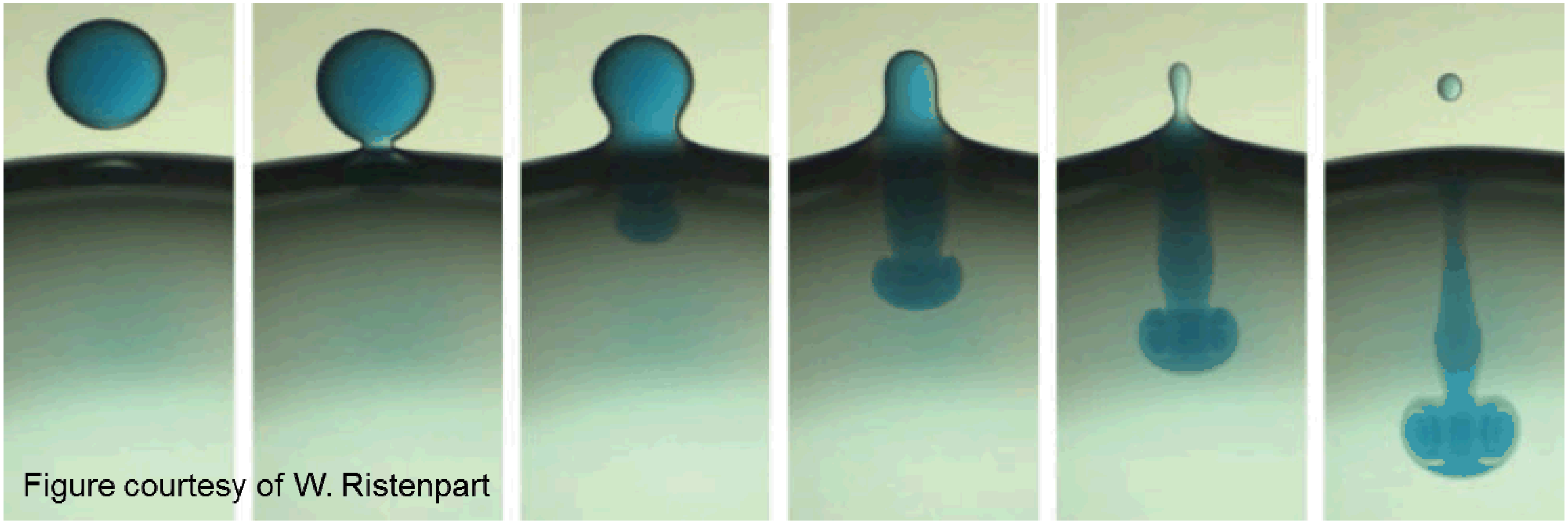
Results: Charge transfer dynamics

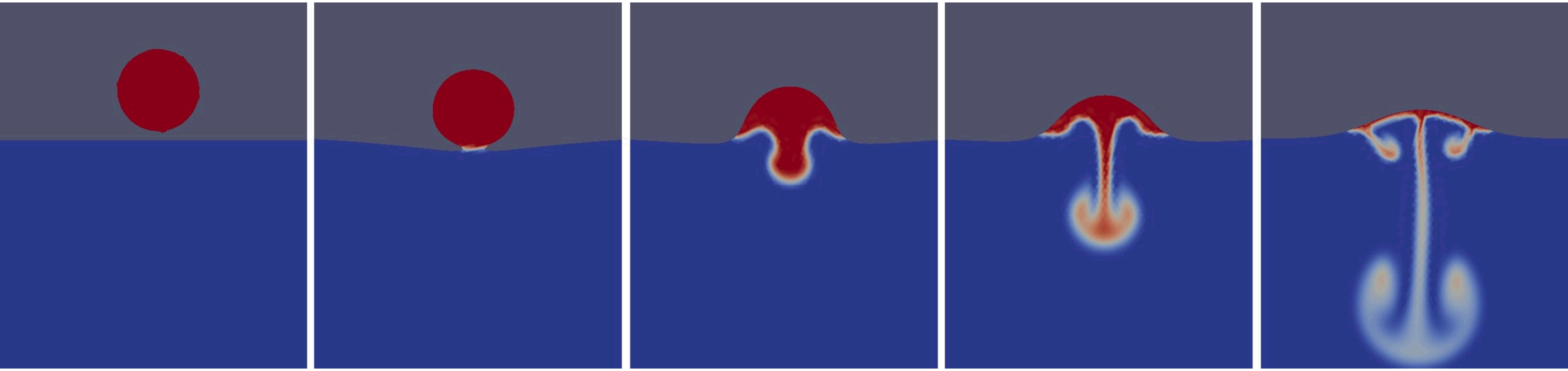
- Droplet contact is very sensitive to mesh geometry
- Cone angle is an important factor in coalescence versus pinch-off





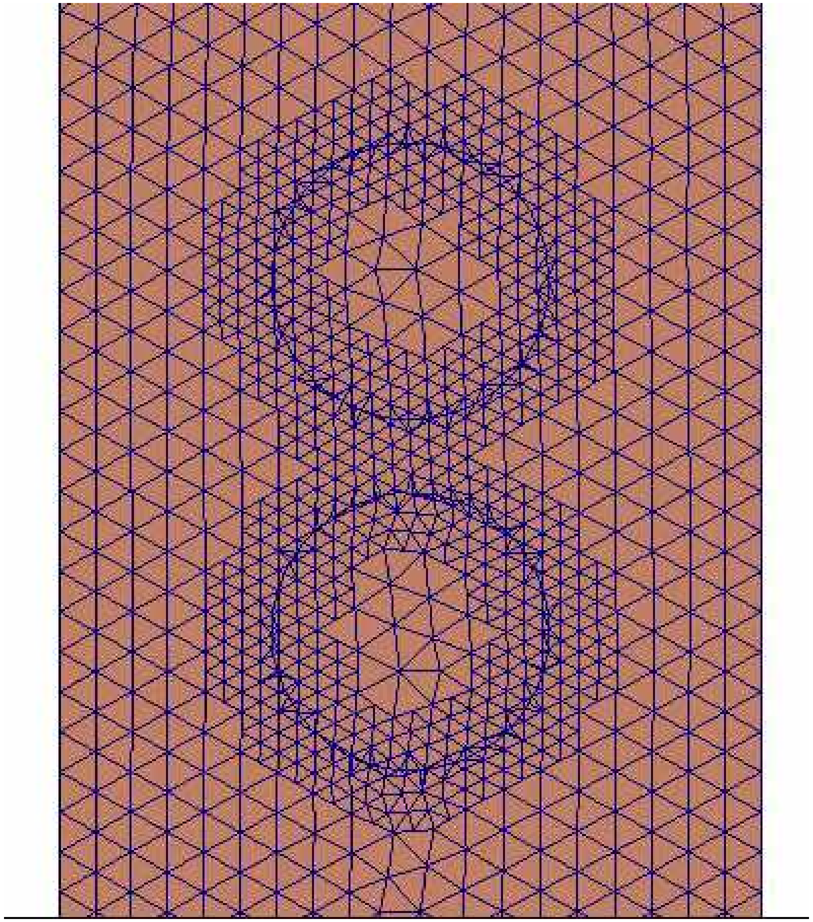
Capturing convective vortices with CDFEM





CDFEM: adaptive mesh refinement

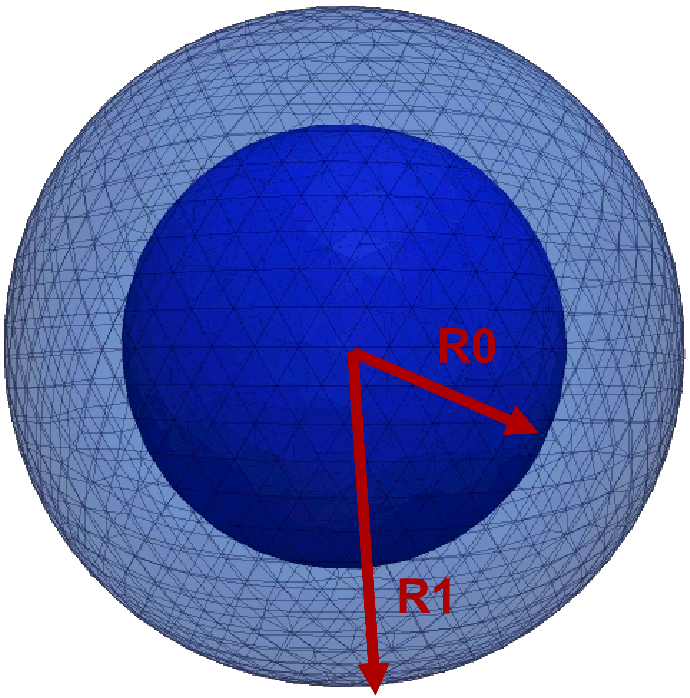
- Mesh can be adaptively refined near the interface to improve accuracy without refining whole mesh
- Multiple levels of adaptivity possible
- Single, multiple or composite level sets can be used to define interfaces



Charge density verification study

- Radially symmetric analytic solution
- Bulk charge

$$\rho^e(R,t) = \rho_0^e e^{-\sigma t/\varepsilon_d} \quad \text{for} \quad R < R_0$$



- Surface charge

$$q(t) = \frac{1}{3} R_0 \rho_0^e (1 - e^{-\sigma t/\varepsilon_d})$$

- Voltage

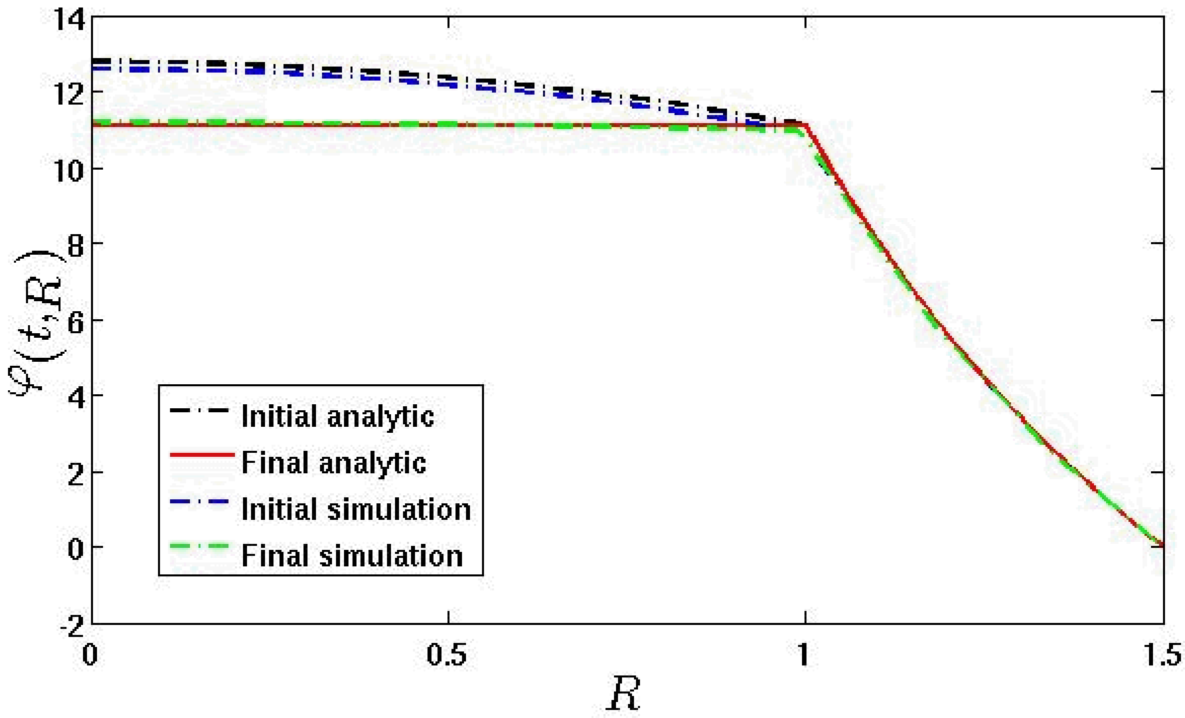
$$R < R_0 \qquad \varphi(R,t) = \frac{\rho_0^e}{6\varepsilon_d}(R_0^2 - R^2)e^{-\sigma t/\varepsilon} + \frac{R_0^3 \rho_0^e}{3\varepsilon_x}\left(\frac{1}{R_0} - \frac{1}{R_1}\right)$$

$$R \geq R_0 \qquad \varphi(R,t) = \frac{R_0^3 \rho_0}{3\varepsilon_x}\left(\frac{1}{R} - \frac{1}{R_1}\right)$$

Charge density verification

- Voltage solutions match well, charge density builds up at interface.
- Works well for stationary problems, but total charge gets lost over time for moving interface
- **(Plan to include plots showing charge loss over time)!**

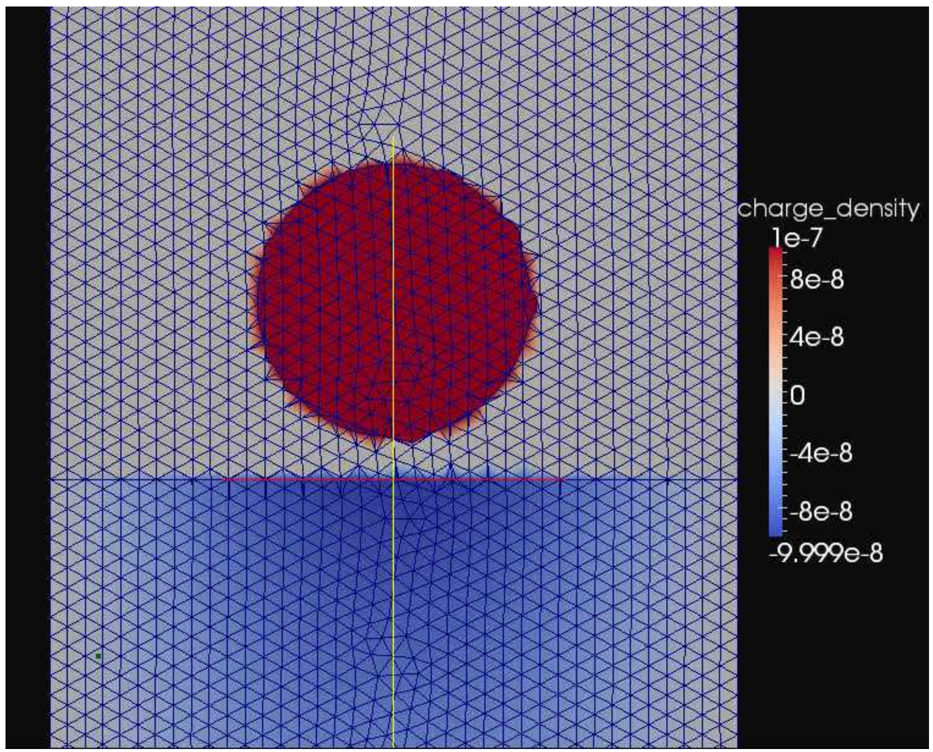
Voltage



Surface charge build-up

- Surface charge equation is necessary in certain parameter regimes

$$\frac{\partial \rho_s}{\partial t} + \boldsymbol{u}\cdot\nabla_s\rho_s - \rho_s\boldsymbol{n}(\boldsymbol{n}\cdot\nabla)\cdot\boldsymbol{u} + |\sigma\boldsymbol{E}\cdot\boldsymbol{n}| = 0 \quad \& \quad |\varepsilon\boldsymbol{E}\cdot\boldsymbol{n}| = \rho_s$$



- Shell element equation for surface charge possible for ALE methods

Summary & future directions

- A sharp, front tracking method (CDFEM) for multi-phase electro-hydrodynamic flows
- Capturing and predicting coalescence requires resolving the charge transfer dynamics near the interface

References:

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BS Hamlin, JC Creasey and WD Ristenpart. Electrically Tunable Partial Coalescence of Oppositely Charged Drops. Phys. Rev. Lett. 109, (2012).