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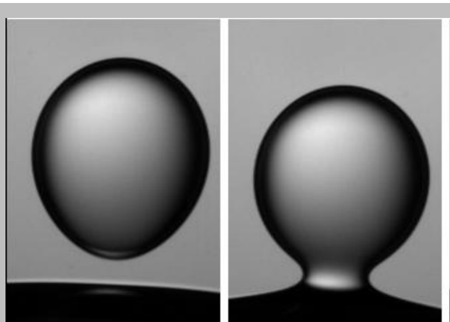

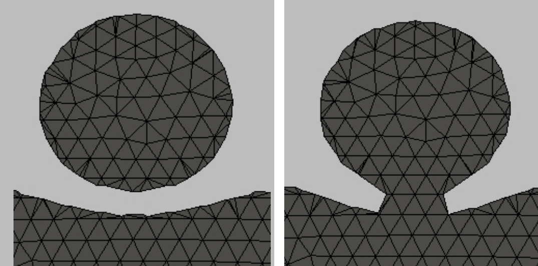

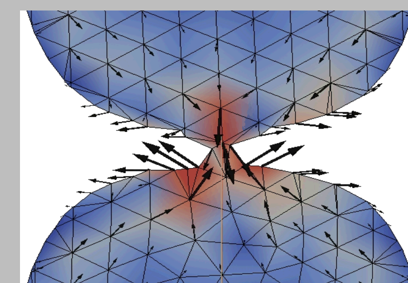

Interface-tracking hydrodynamic model for droplet electro-coalescence

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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

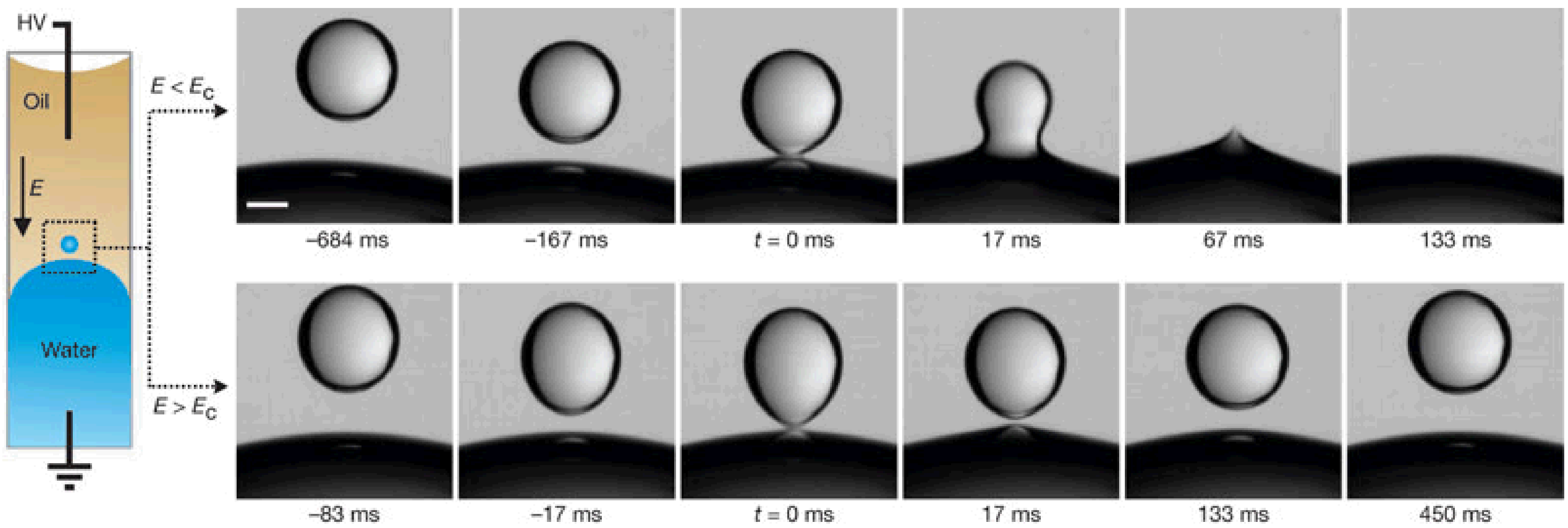


Figure courtesy of W. Ristenpart

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:

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

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

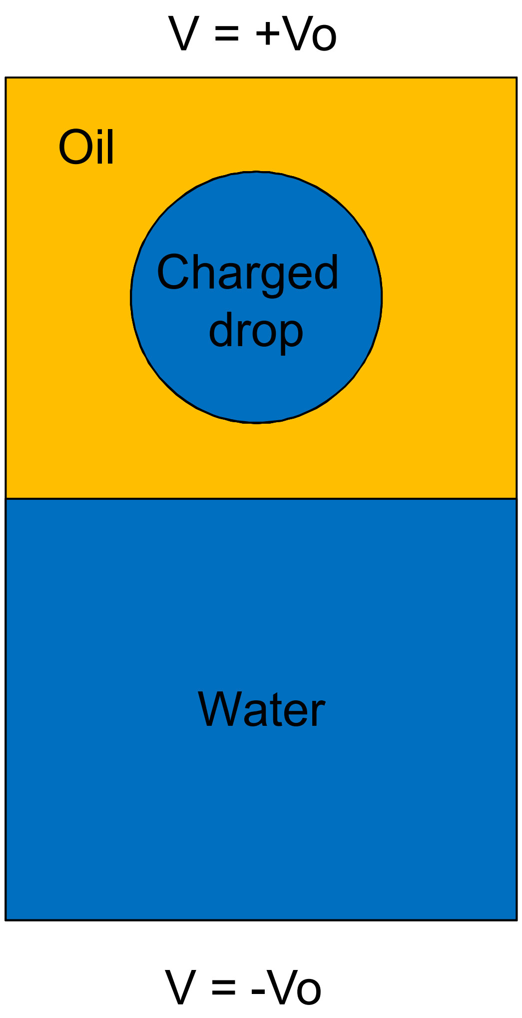
- Force due to electric field (divergence of the Maxwell stress tensor):

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

- Charge density and voltage equations:

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

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



Governing equations

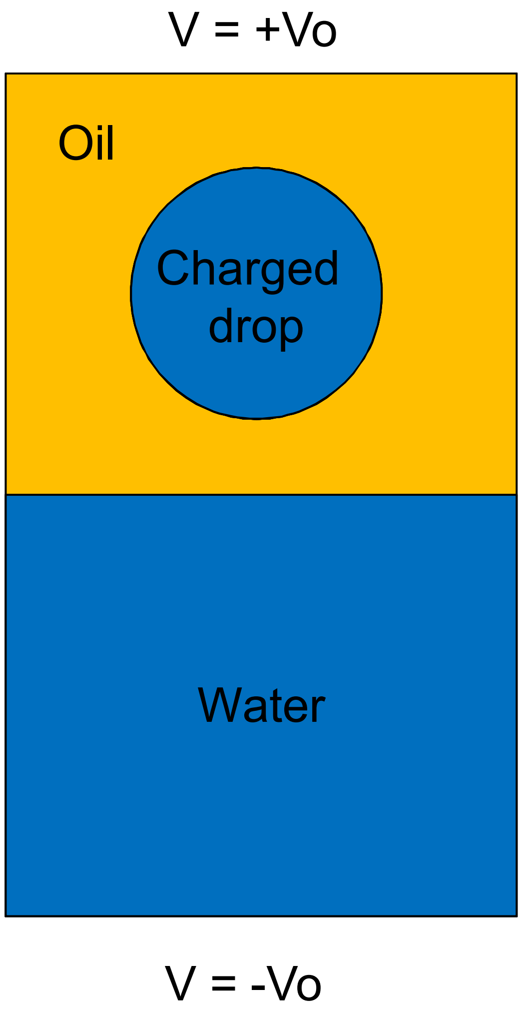
- Level set equation (tracks interface):

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

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

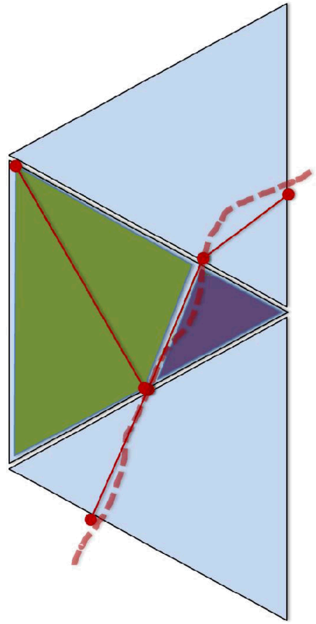
- Surface charge equation:

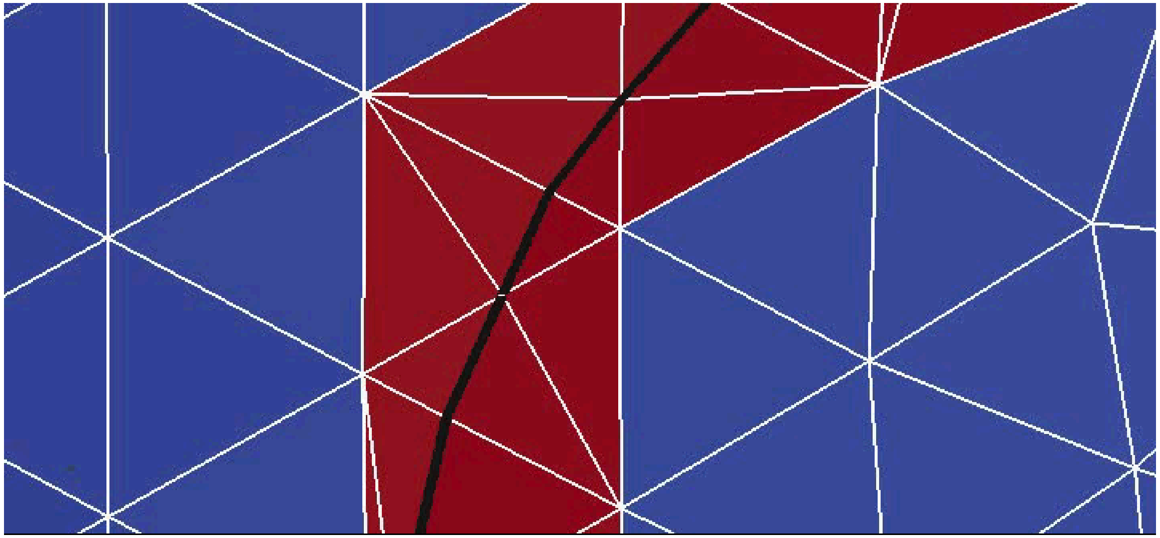
$$\frac{\partial \rho_s}{\partial t} + \boldsymbol{u} \cdot \nabla_s \rho_s - \rho_s \boldsymbol{n}(\boldsymbol{n} \cdot \nabla) \cdot \boldsymbol{u} + \lfloor \sigma \boldsymbol{E} \cdot \boldsymbol{n} \rfloor = 0$$



CDFEM: an interface-tracking method

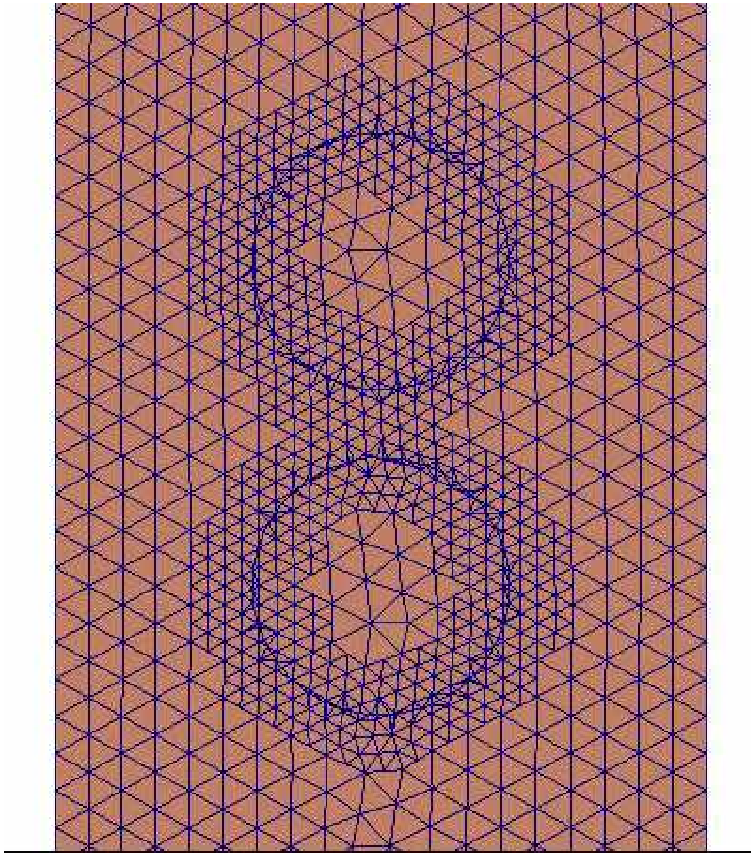
- Conformal decomposition finite element method (CDFEM)
- Sharp interface method that dynamically cuts elements at interface (tri/tet)
- Interface tracked by one or more level set functions





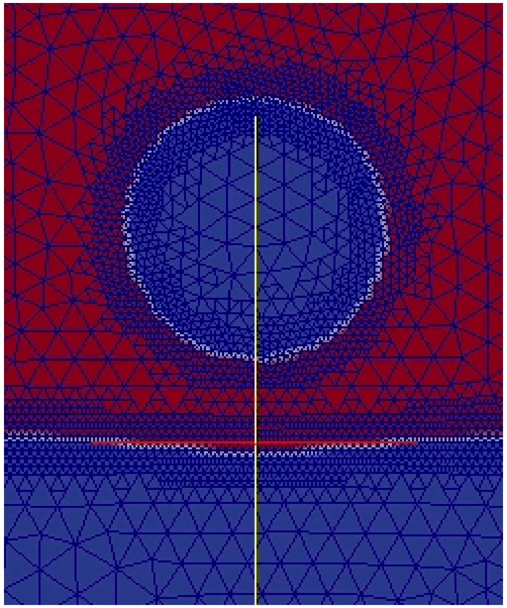
CDFEM: an interface-tracking method

- Mesh can be adaptively refined near the interface
- Multiple levels of adaptivity possible
- Single, multiple or composite level sets can define interfaces

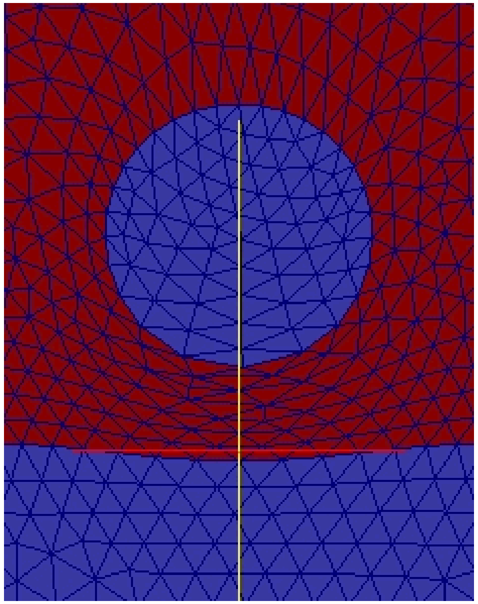


Method comparison

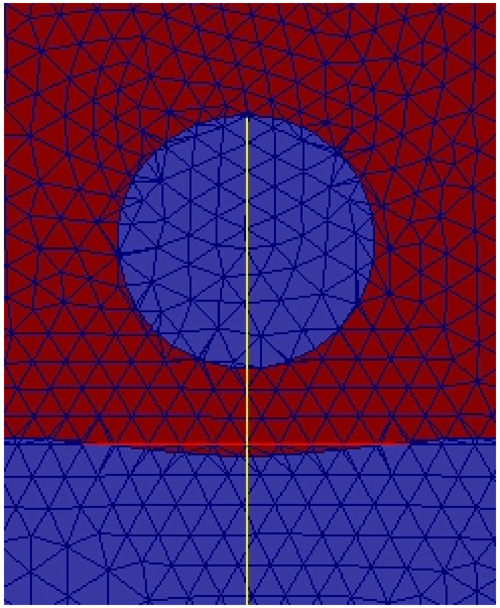
- Diffuse level set – interface gets smeared
- ALE (Arbitrary Lagrangian Eulerian)– elements need to be deleted/added as droplet merges
- CDFEM – minimal new elements created (however a tri/tet mesh necessary for decomposition algorithm)



Diffuse level set



ALE



CDFEM

Results: droplet deformation

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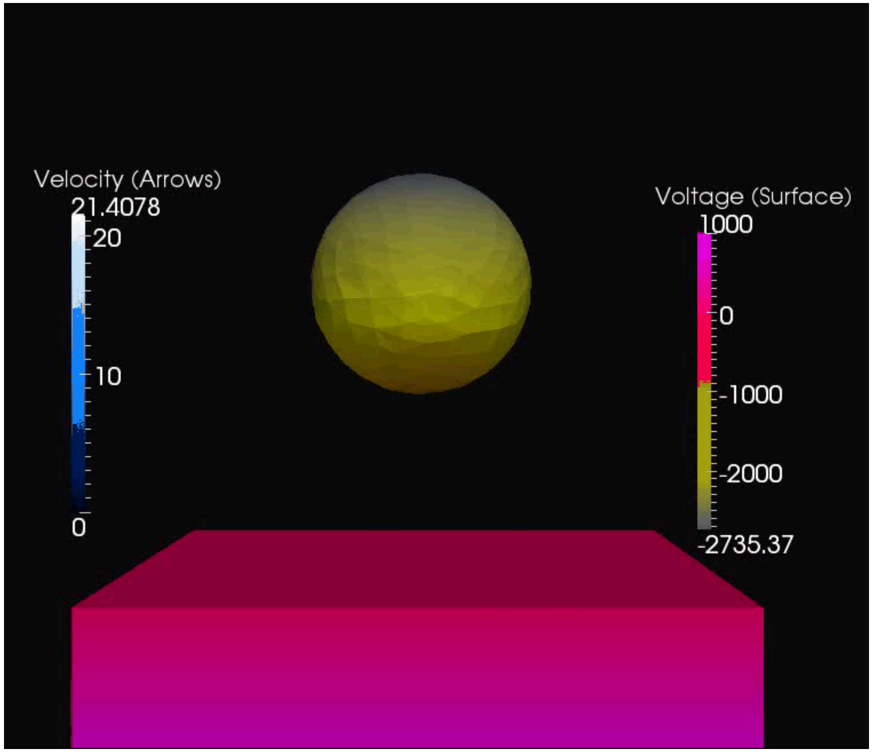
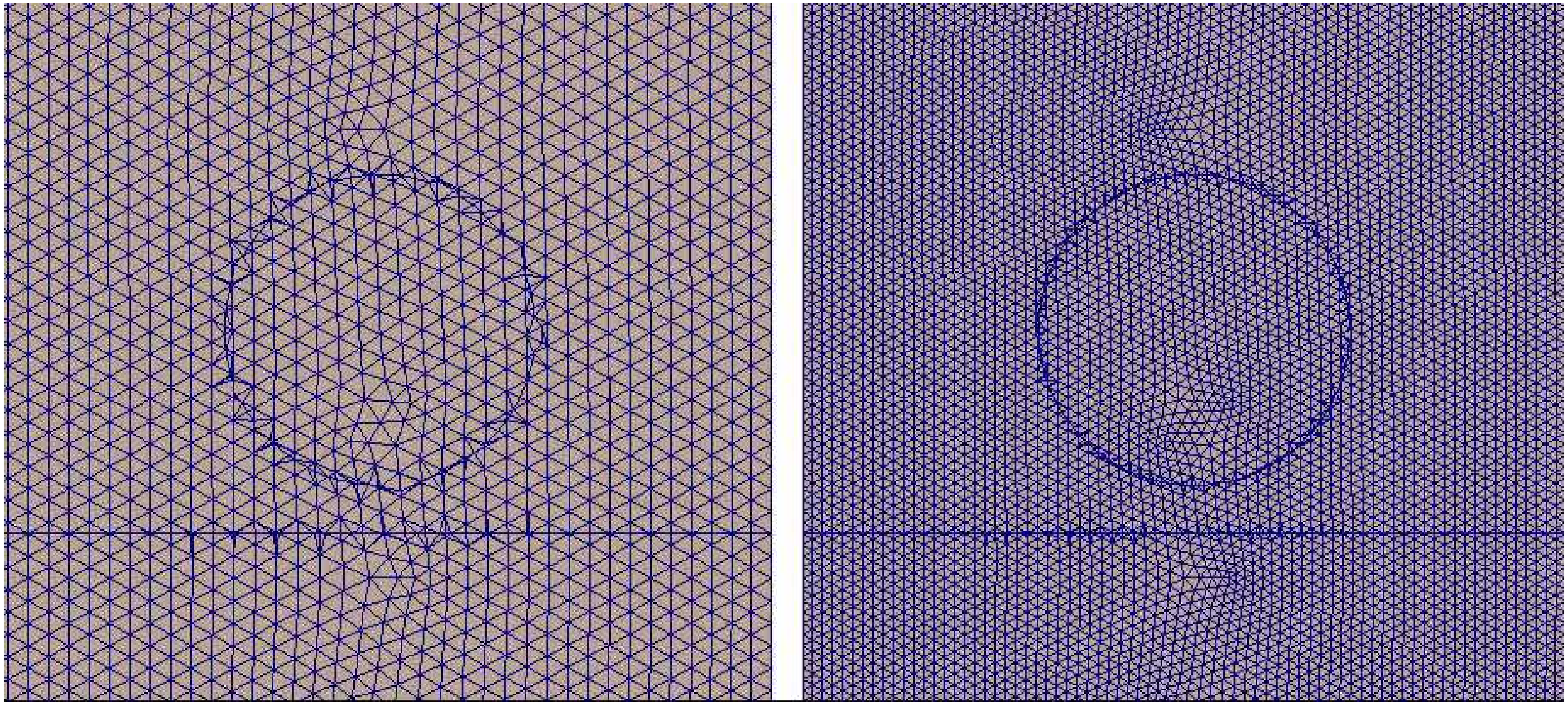
- Simulation of a 3D droplet deforming under electric field via a jump in permittivity between phases



Grid refinement study for coalescence

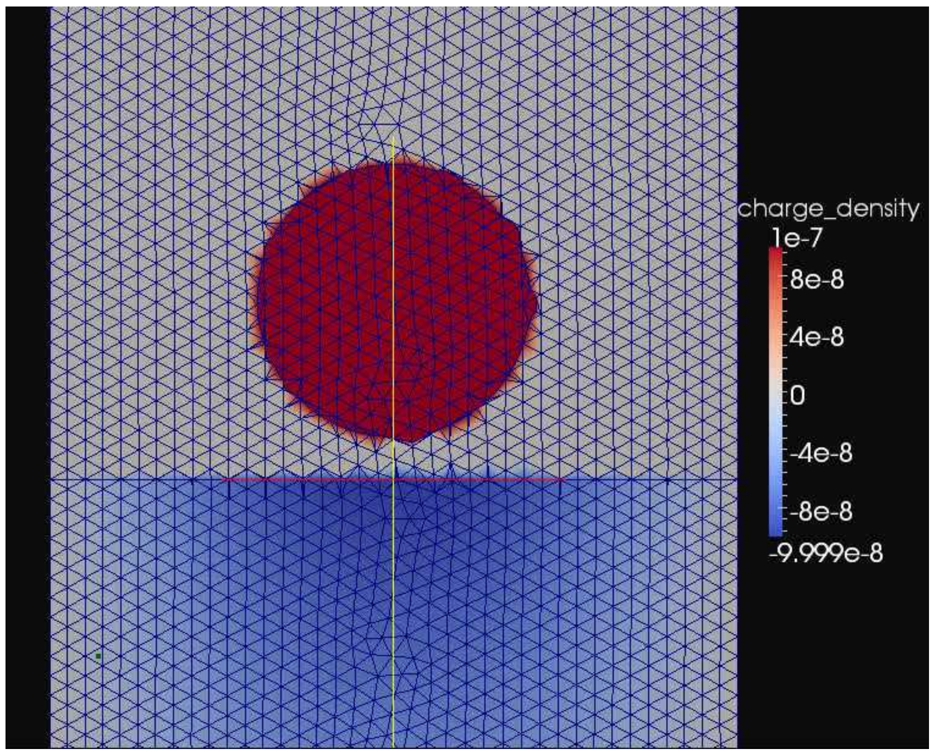
- Coalescence is a function of mesh width
  - Adaptive mesh refinement and adaptive time stepping
  - Multi-scale method



Surface charge build-up

- Surface charge equation is necessary in certain parameter regimes

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



- Surface equation not implemented in code yet

Summary & future directions

- A sharp, front tracking method (CDFEM) for multi-phase electro-hydrodynamic flows
- Capturing and predicting coalescence requires solving surface charge density equation at the interface as well as in the bulk – charge transfer dynamics are very important

References:

DR Noble, EP Newren and JB Lechman. A conformal decomposition finite element method for modeling stationary fluid interface problems. *International Journal for Numerical Methods in Fluids* (2010): **63**, pp. 725-742.

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WD Ristenpart, JC Bird, A Belmonte, F Dollar and HA Stone. Non-coalescence of oppositely charged drops. *Nature* (2009): **461**, pp 377-380.