A phase field model for the coupling between Navier-Stokes and electrokinetic equations

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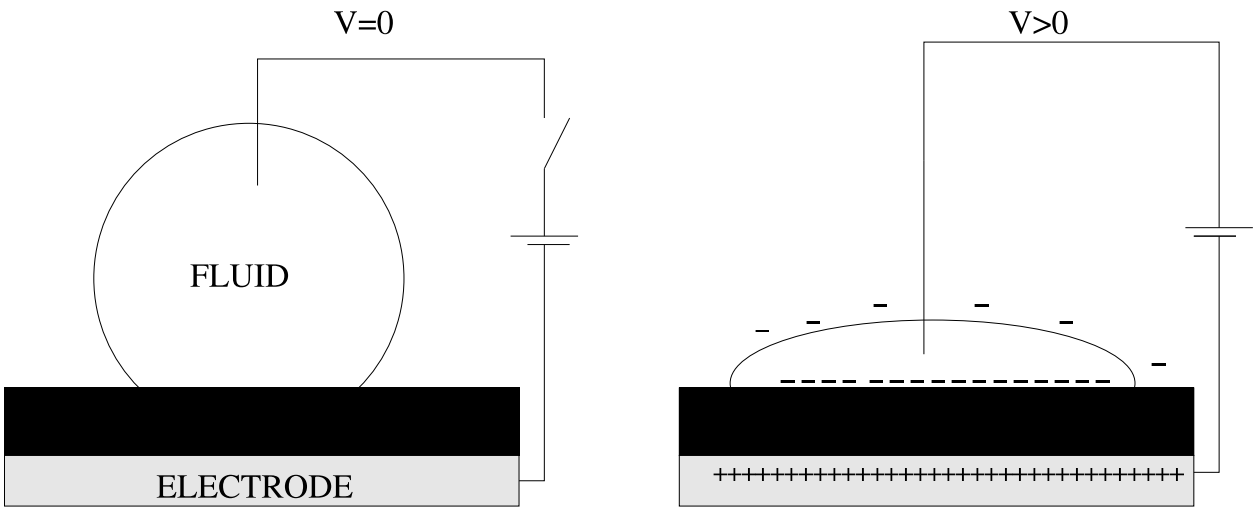
Outline

1) Motivation: Electrowetting and Rayleigh jets
2) Phase fields
3) Coupling of Navier-Stokes, Poisson and Electrokinetic equations through a phase field
4) Existence theorem
5) Numerical implementation

Electrowetting

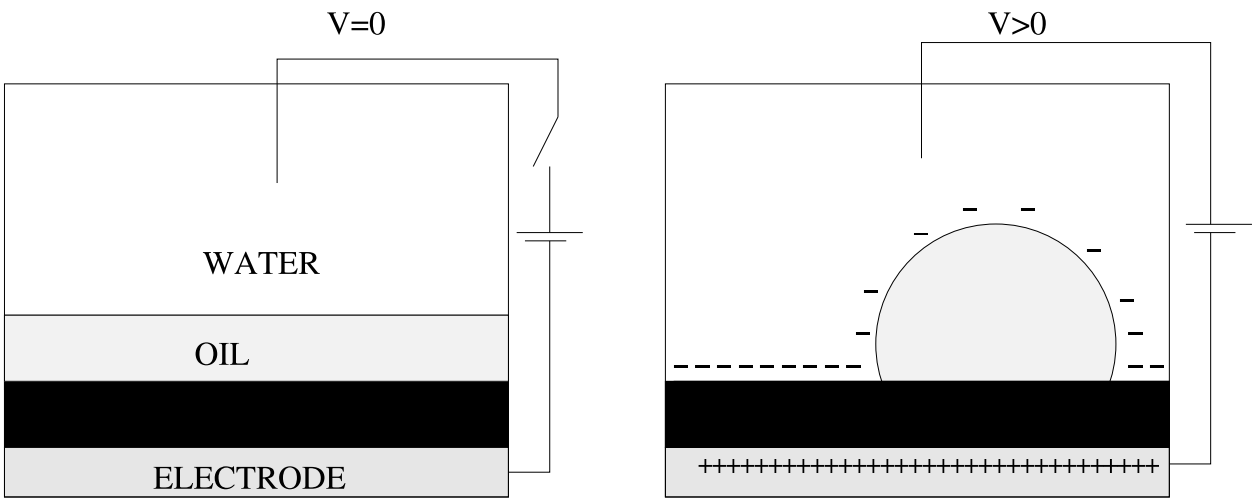
Aim: Modify wetting behaviour, shape, movement of liquid droplets by application of electric charges / voltages



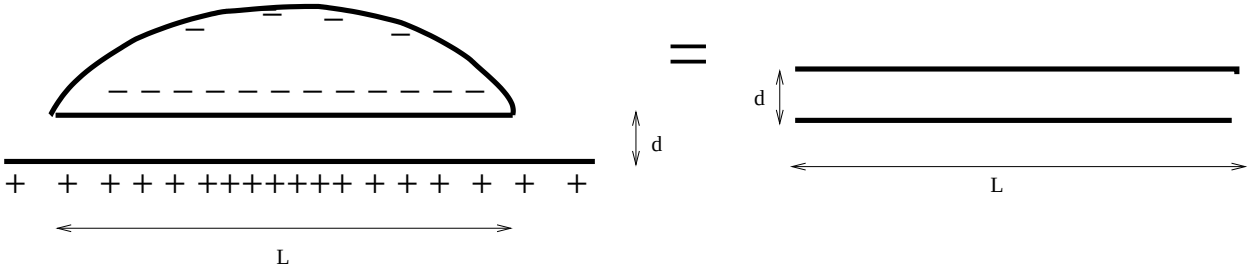
Droplet: electrically conductive liquid, surrounded by insulating gas or fluid

Applications

- pixelated optical filters
- adaptive lenses
- curtain coating
- fast switching electrowetting displays



Phase field model



$$E = \gamma_{lg} A_{lg} + \gamma_{ls} A_{ls} + \gamma_{gs} A_{gs} - \frac{1}{2} Q V$$

Phase field model

$$
\begin{aligned}
E &= \gamma_{lg} A_{lg} + \gamma_{ls} A_{ls} + \gamma_{gs} A_{gs} - \frac{1}{2} QV \\
&= \gamma_{gs}(A_{ls} + A_{gs}) + \gamma_{lg} A_{lg} + (\gamma_{ls} - \gamma_{gs}) A_{ls} - \frac{1}{2} QV \\
&= E_0 + \gamma_{lg} \left(A_{lg} + \frac{\gamma_{ls} - \gamma_{gs}}{\gamma_{lg}} A_{ls} - \frac{1}{2\gamma_{lg}} QV \right) \\
&= E_0 + \gamma_{lg} \left(A_{lg} - (\cos\theta_Y) A_{ls} - \frac{1}{2\gamma_{lg}} QV \right)
\end{aligned}
$$

$$
QV = CV^2 = CV^2 \simeq \frac{\varepsilon}{d} A_{ls} V^2
$$

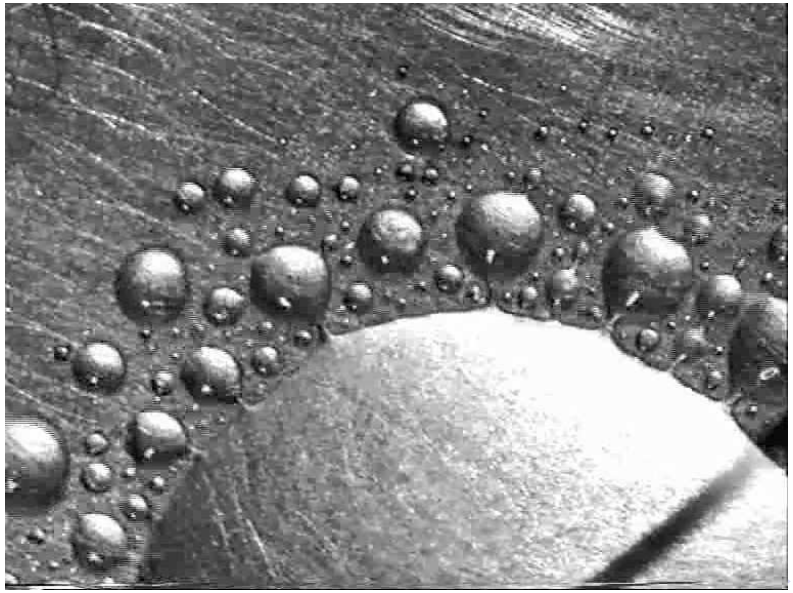
$$
\cos\theta(V) = \cos\theta_Y + \frac{\varepsilon}{2d\gamma_{lg}} V^2
$$

Phase field model

G. Lippmann (1875): Decrease of contact angle with the applied potential. Lippmann-Young eqn.

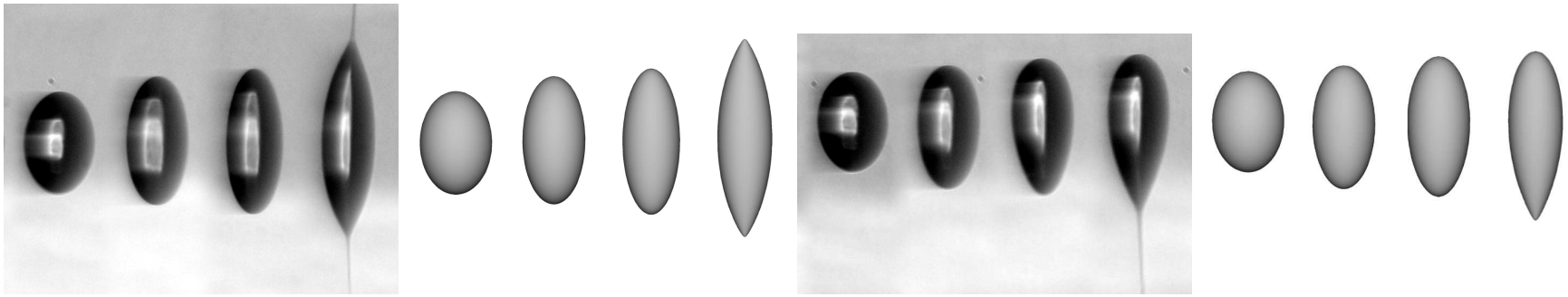
$$\cos\theta(V) = \cos\theta_Y + \frac{\varepsilon}{2d\gamma_{\mathrm{lg}}}V^2$$

Contact angle saturation and contact line instability



Rayleigh Jets

Bursting of charged drops in an electric field
Rayleigh 1882, Duft et al. 2003



Singularity development if one uses Navier-Stokes with classical boundary conditions for perfectly conductive medium ,Betelú, F.,Kindelán, Vantzos 2007

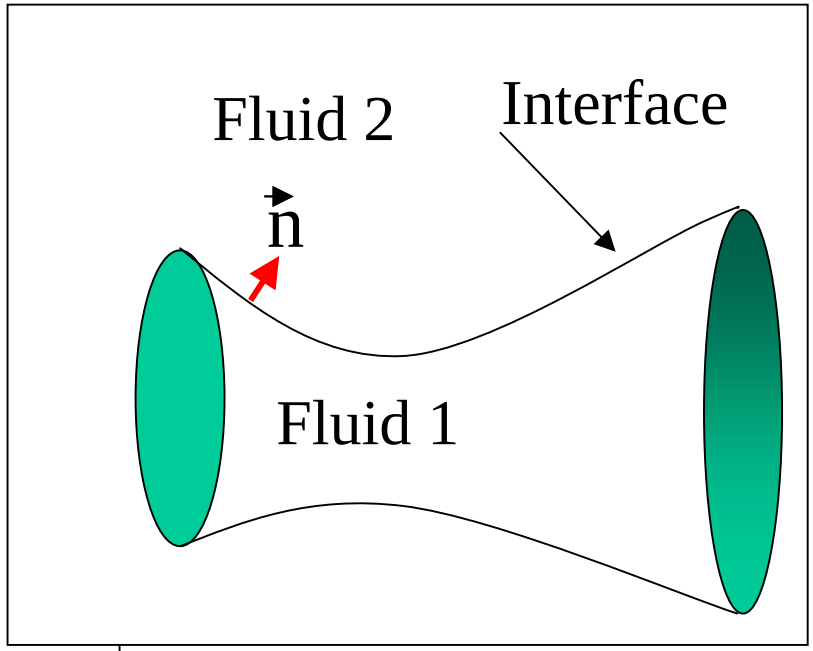
Strong dependence of jet's diameter and velocity on Electrical conductivity

Fluid 1

$$\rho_1 \left(\frac{\partial \mathbf{v}^{(1)}}{\partial t} + \left(\mathbf{v}^{(1)} \cdot \nabla \right) \mathbf{v}^{(1)} \right) = \nabla \cdot \boldsymbol{\sigma}^{(1)} + \mathbf{F}$$

$$\nabla \cdot \mathbf{v}^{(1)} = 0$$

$$\boldsymbol{\sigma}_{ij}^{(1)} = -p^{(1)} \delta_{ij} + \mu_1 \left(v_{i,j}^{(1)} + v_{j,i}^{(1)} \right)$$



Fluid 2

$$\rho_2 \left(\frac{\partial \mathbf{v}^{(2)}}{\partial t} + \left(\mathbf{v}^{(2)} \cdot \nabla \right) \mathbf{v}^{(2)} \right) = \nabla \cdot \boldsymbol{\sigma}^{(2)} + \mathbf{F}$$

$$\nabla \cdot \mathbf{v}^{(2)} = 0$$

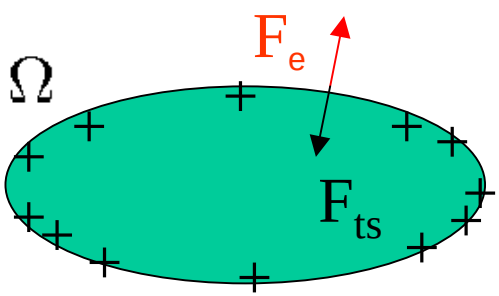
$$\boldsymbol{\sigma}_{ij}^{(2)} = -p^{(2)} \delta_{ij} + \mu_2 \left(v_{i,j}^{(2)} + v_{j,i}^{(2)} \right)$$

Interface

$$\left[\boldsymbol{\sigma}^{(2)} - \boldsymbol{\sigma}^{(1)} \right] \mathbf{n} = F_s \ \mathbf{n}$$

$$\mathbf{v}^{(1)} = \mathbf{v}^{(2)} = \mathbf{v}$$

$$V_N = \mathbf{v} \cdot \mathbf{n}$$



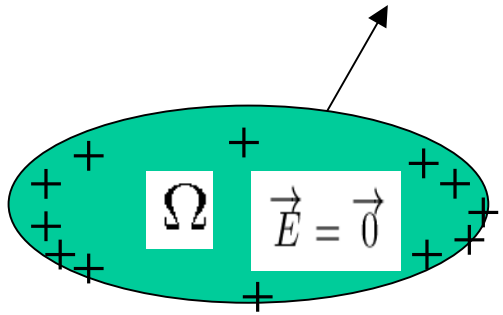
$$F_s \vec{n} = \left(\gamma\kappa - \frac{\sigma^2}{2\varepsilon_0}\right)\vec{n} \text{ on } \partial\Omega(t)$$

$$\sigma = \varepsilon_0 E_n$$

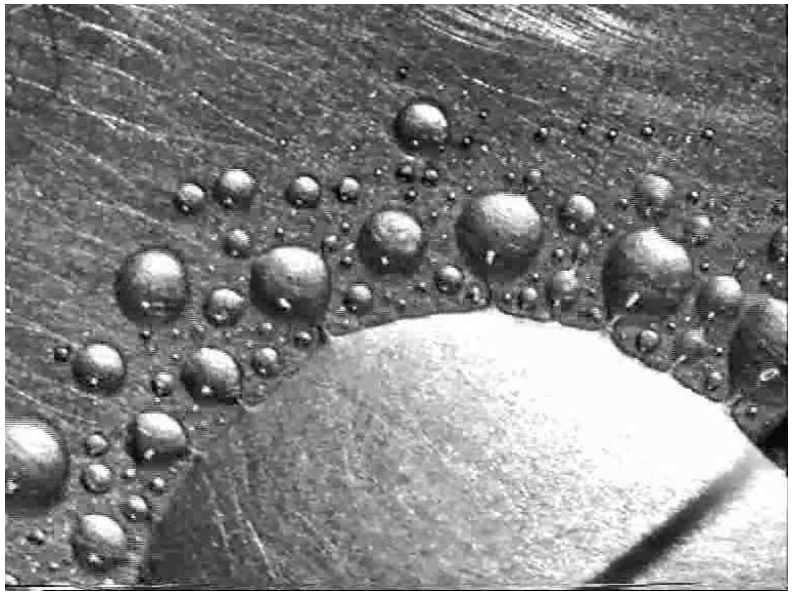
2.1 ELECTRIC FIELD EQUATIONS

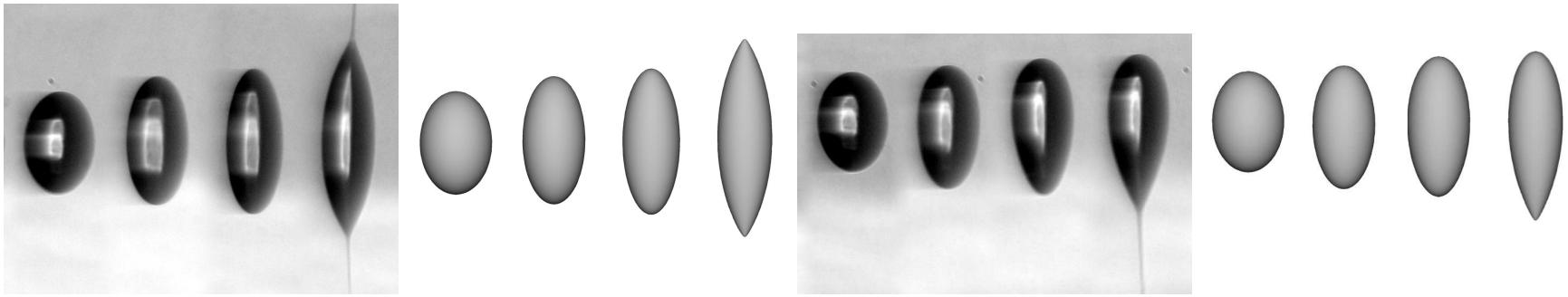
$$\begin{aligned} \Delta V &= 0 \text{ in } \mathbb{R}^3 \backslash \Omega \,, \\ V &= C \text{ on } \partial\Omega \,, \\ V(\mathbf{r}) &\to 0 \text{ when } |\mathbf{r}| \to \infty \,, \\ \vec{E} &= \vec{0} \text{ in } \Omega \left(\vec{E} = \nabla V\right) \end{aligned}$$

Conductor: $V = C$



Dielectric: $\Delta V = 0$



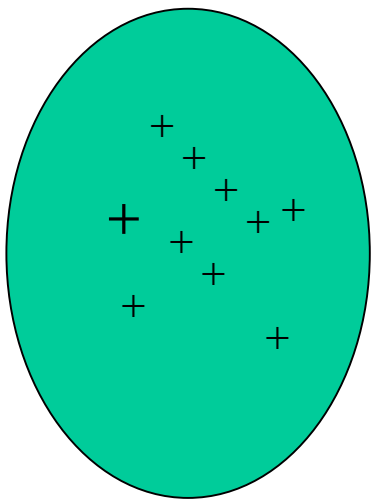


Are the satellite droplets and Rayleigh jets due to finite electrical conductivity?(our conjecture)

ELECTROKINETIC EQUATION

Volumetric

Charge density ρ



$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = \nabla \cdot \left(-K\vec{E} + D\nabla\rho\right)}$$

Convective flux

$$\vec{J} = -K\vec{E} + D\nabla\rho$$

Diffusive flux

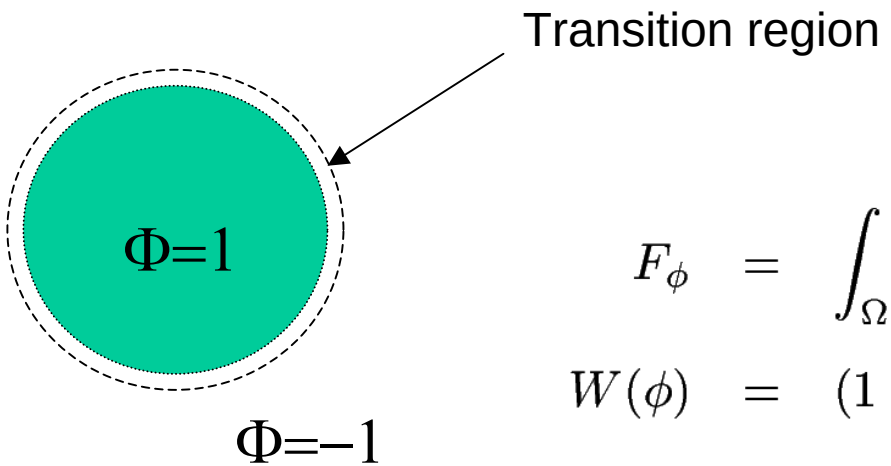
Ohm's law (drift)

$$\boxed{-\nabla \cdot (\varepsilon \nabla V) = \rho}$$

K, D, μ, ε depend now on x

Problem: No clear boundary condition for V and hence no clear boundary condition for Navier-Stokes. We have to deal with the two fluids simultaneously and (somehow) ignore the presence of a boundary.

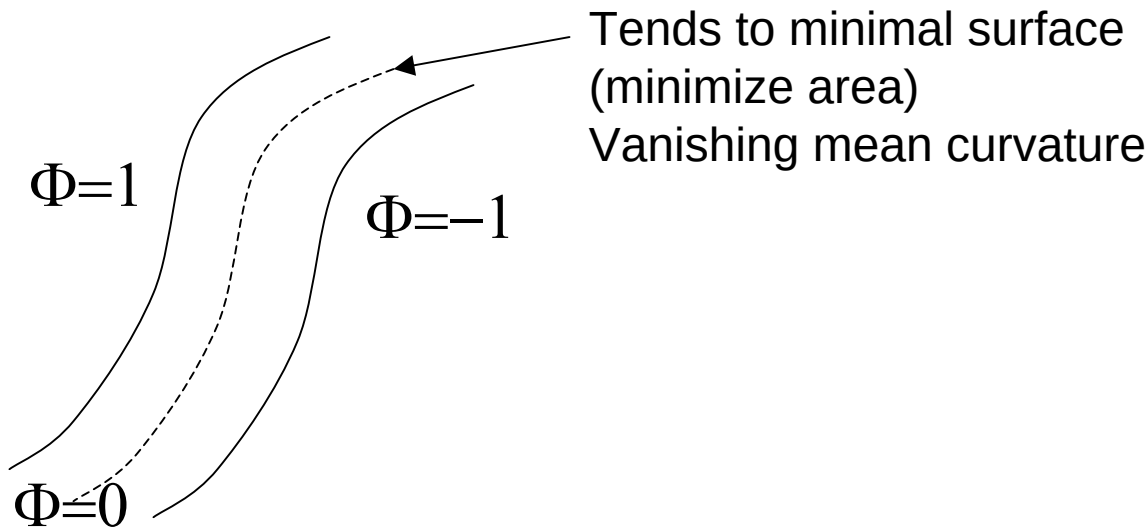
Minimal surfaces



$$F_\phi = \int_\Omega \left(\delta \frac{|\nabla \phi|^2}{2} + \frac{W(\phi)}{\delta} \right) dx \ , \quad \delta \ll 1$$

$$W(\phi) = (1-\phi^2)^2$$

$$\boxed{Min\,(F_\phi) \Rightarrow -\delta^2 \Delta \phi + W'(\phi) = 0}$$



N-S with surface tension: $$\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} = -\nabla p + \nu \Delta \vec{v} + \gamma \kappa \delta_S$$

Possible formulation of Navier-Stokes:

$$\boxed{\begin{aligned} &\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} = -\nabla p + \nu \Delta \vec{v} + \frac{\gamma}{2} \mu \nabla \phi \\ &\mu = -\delta \Delta \phi + \frac{W'(\phi)}{\delta} \ , \quad (M \quad mobility) \end{aligned}}$$

Conservation of total mass: $\int_\Omega \phi dx \quad = \quad Const.$

Recover stationary. Config.: $\mu \quad \simeq \quad C$

$$\boxed{\frac{\partial \phi}{\partial t} + \nabla \cdot (\vec{v} \phi) = \nabla \cdot (M \nabla \mu) \ , \quad Cahn - Hilliard}$$

Existence of weak solutions: Feng, Abels, 2006

Important open problem: Do we recover the solutions of NS with surface tension when δ tends to zero?

Remark: in reality both viscosity and mobility should depend on Φ

$$\boxed{\begin{aligned} \frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} &= -\nabla p + div\left(\frac{\nu(\phi)}{2}(\nabla \vec{v} + (\nabla \vec{v})^T)\right) + \frac{\gamma}{2}\mu \nabla \phi \ , \\ \frac{\partial \phi}{\partial t} + \nabla \cdot (\vec{v}\phi) &= \nabla \cdot (M(\phi)\nabla \mu) \ . \end{aligned}}$$

Important advantages:
-No need to implement boundary conditions in a free boundary.
-We can handle topological changes (collapse or snap-off of drops).

Minor drawbacks:
- Not a well developed mathematical analysis (YET),
- Numerically expensive (Cahn-Hilliard is 4th order).

The model

Features:

- Movement of fluids/gases: Stokes–System
- Movement of interface between fluids (or fluid and gas): phase field model of Cahn–Hilliard type
- Electric field: potential equation
- Transport of electric charges: Ohms law
  Conductivity nonzero in droplet only
  Charges accumulate at interface, smoothing by diffusion

Variational principle (Onsager)

$$\boxed{D_{\mathbf{J}}\left(\frac{d}{dt}F(\mathbf{J}) - \Phi(\mathbf{J},\mathbf{J})\right) = 0}$$

F — free energy
Φ — dissipation function
$\mathbf{J}$ — generalized fluxes

Free energy

$$\mathscr{F} = \underbrace{\int_\Omega \left(\frac{\delta}{2}|\nabla\phi|^2 + \frac{W(\phi)}{\delta} \right) dx}_{\text{surface energy of phase field model}} + \underbrace{\int_\Gamma \gamma_{fs}(\phi)\, ds}_{\substack{\text{interfacial energy} \\ \text{liquid–solid}}}$$

$$+ \underbrace{\frac{1}{2}\int_\Omega \frac{|\boldsymbol{D}|^2}{\varepsilon(\phi)}\, dx}_{\text{energy of electric field}} + \underbrace{\frac{\lambda}{2}\int_\Omega \rho^2\, dx}_{\substack{\text{smoothing of} \\ \text{surface charge}}}$$

γ_{fs} — fluid–solid interface energy
$\boldsymbol{D} = \varepsilon(\phi)\boldsymbol{E}$ — dielectric displacement
$\boldsymbol{E} = -\nabla U$ — electric field, U — electric potential

Dissipation function

$$\Phi(\mathbf{J},\mathbf{J}) = \int_\Omega \frac{|\boldsymbol{J}_\phi|^2}{2M(\phi)}\,dx + \int_\Gamma \frac{(d_t\phi)^2}{2\alpha^{-1}}\,ds + \int_\Omega \frac{|\boldsymbol{J}_{\boldsymbol{D}}|^2}{2K(\phi)}\,dx$$
$$+ \int_\Omega \eta(\phi)\frac{|\boldsymbol{T}(\boldsymbol{v})|^2}{2}\,dx + \int_\Gamma \frac{\beta}{2}|\boldsymbol{v}_\tau|^2\,ds$$

$\mathbf{J} = (\boldsymbol{v}, d_t\phi, \boldsymbol{J}_\phi, \boldsymbol{J}_{\boldsymbol{D}})$ — generalized fluxes

d_t — material time derivative

M — mobility

η — viscosity

α — kinetic parameter

$\boldsymbol{T}(\boldsymbol{v}) = \frac{1}{2}\left(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^\top\right)$ — velocity strain tensor

β — friction parameter

Variational principle $\Rightarrow$ Constitutive equations for fluxes

$$\boldsymbol{J}_\phi = -M(\phi)\nabla\mu$$
$$\boldsymbol{J}_{\boldsymbol{D}} = K(\phi)(\boldsymbol{E} - \lambda\nabla\rho)$$

with chemical potential $\mu = \underbrace{-\delta\Delta\phi + \frac{1}{\delta}W(\phi)}_{\text{surface tension}} - \underbrace{\frac{1}{2}\varepsilon'(\phi)|\nabla U|^2}_{\text{ponderomotive force}}$

Boundary conditions for phase field:

$$-\alpha\, d_t\phi = \left(\gamma'_{fs}(\phi) + \delta\frac{\partial\phi}{\partial n}\right)$$

Stokes–system for velocity

$$-\nabla \cdot (\eta(\phi)\boldsymbol{T}(\boldsymbol{v})) - \mu\nabla\phi - \rho\boldsymbol{E} + \nabla p = 0 \text{ in } \Omega$$
$$\boldsymbol{v} = 0 \;\text{ or }\; \beta\boldsymbol{v}_\tau + \eta(\phi)(T(\boldsymbol{v})\boldsymbol{n})_\tau = -\alpha\, \boldsymbol{d}_t\phi\, \partial_\tau\phi \text{ on } \partial\Omega$$

Equation for phase field

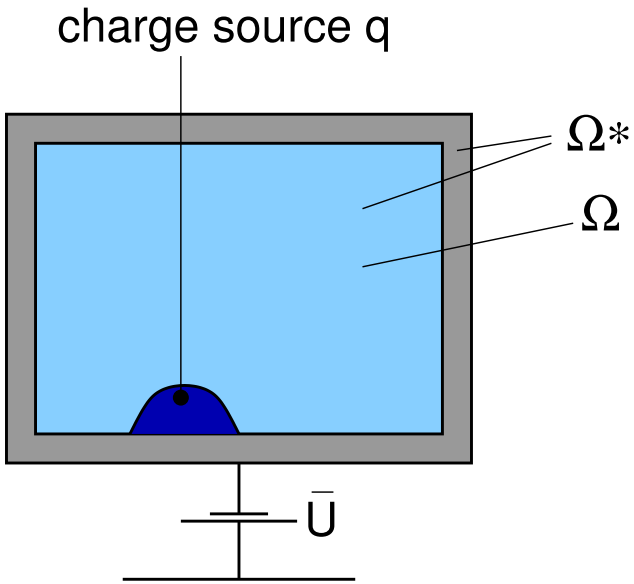
$$\partial_t\phi + \nabla \cdot (\phi\boldsymbol{v}) = \nabla \cdot \boldsymbol{J}_\phi$$

Equations for charge transport:

$$\partial_t\boldsymbol{D} = \boldsymbol{J}_{\boldsymbol{D}}$$
$$\nabla \cdot \boldsymbol{D} = \rho$$

Analysis

Geometry



$\boldsymbol{v}$, ϕ, μ, ρ in Ω
U in Ω^*
$U = \overline{U}$ on $\partial\Omega^*$
Charge source q in Ω

Result: Existence of weak solutions for no–slip boundary condition $v = 0$ and

- non–degenerate electric conductivity $K(\phi) \geq k_0 > 0$ or
- degenerate conductivity, constant electric permittivity ε

Theorem: there exist global in time weak solutions to the system.

Weak formulation

Function spaces:

$$\mathcal{V} := \{v \in H^1(\Omega) \,|\, \nabla \cdot v = 0\}$$

for velocity field,

$$\mathcal{W} := H^1(\Omega)$$

for ρ, ϕ, μ, and

$$\mathcal{U} := H_0^1(\Omega^*)$$

for potential $u = U$.

Find $v \in L_2(I;\mathcal{V})$, $\rho, \phi, \mu \in L_2(I;\mathcal{W})$, $U \in L_\infty(I;\mathcal{U})$ *with* $\rho, \phi \in H^1(I;\mathcal{W}^*)$, $\rho(0,\cdot) = \rho_0$, $\phi(0,\cdot) = \phi_0$ *such that for every* $w \in \mathcal{V}$, $\psi \in \mathcal{W}$, $\chi \in \mathcal{U}$ *and almost every time* t *the following equations are true:*

Weak formulation

$$\int_\Omega \big(\eta(\phi)T(\boldsymbol{v}) : T(\boldsymbol{w}) - \mu\,\nabla\phi\cdot\boldsymbol{w} + \rho\,\nabla U\cdot\boldsymbol{w}\big)\,dx = 0$$

$$\int_\Omega \big(\partial_t\rho\,\psi + \boldsymbol{v}\cdot\nabla\rho\,\psi + K(\phi)\nabla(U+\lambda\rho)\cdot\nabla\psi\big)\,dx = \int_\Omega q\,\psi\,dx$$

$$\int_\Omega \big(\partial_t\phi\,\psi + \boldsymbol{v}\cdot\nabla\phi\,\psi + M(\phi)\nabla\mu\cdot\nabla\psi\big)\,dx = 0$$

$$\int_\Omega \mu\,\psi\,dx = \int_\Gamma \big(\alpha\,\partial_t\phi + \gamma'_{fs}(\phi)\big)\psi\,ds + \int_\Omega \big(\delta\nabla\phi\cdot\nabla\psi + \tfrac{1}{\delta}W'(\phi)\,\psi - \tfrac{1}{2}\varepsilon'(\phi)|\nabla U|^2\psi\big)\,dx$$

$$\int_{\Omega^*} \varepsilon(\phi)\nabla U\cdot\nabla\chi\,dx = \int_\Omega \rho\,\chi\,dx$$

A priori estimate

$$
\begin{aligned}
&\frac{d}{dt}\left[\int_\Omega \left(\frac{1}{2}\rho^2 + \frac{\delta}{2}|\nabla\phi|^2 + \frac{1}{\delta}W(\phi)\right)\,dx + \int_{\Omega^*} \frac{\varepsilon(\phi)}{2}|\nabla U|^2\,dx\right] \\
&\quad + \int_\Omega \left[\eta(\phi)|T(\boldsymbol{v})|^2 + K(\phi)|\nabla(U+\lambda\rho)|^2 + M(\phi)|\nabla\mu|^2\right]\,dx \\
&\quad + \frac{d}{dt}\int_\Gamma \gamma_{fs}(\phi)\,ds + \int_\Gamma \alpha|\partial_t\phi|^2\,ds \\
&= \int_\Omega q(U+\lambda\rho)\,dx + \int_{\Omega^*} \varepsilon(\phi)\nabla U\cdot\nabla\overline{U}\,dx
\end{aligned}
$$

We use finite dimensional subspaces

$$
\begin{aligned}
V_n &:= \{w_1, w_2, w_3, \ldots, w_n\} \quad \text{of } \mathcal{V}, \\
W_n &:= \{\psi_1, \psi_2, \psi_3, \ldots, \psi_n\} \quad \text{of } \mathcal{W}, \\
U_n &:= \{\chi_1, \chi_2, \chi_3, \ldots, \chi_n\} \quad \text{of } \mathcal{U}
\end{aligned}
$$

and look for solutions

$$
\begin{aligned}
v(t,x) \sim v^{(n)}(t,x) &:= \sum_{j=1}^{n} v_j(t)\, w_j(x), \\
\rho(t,x) \sim \rho^{(n)}(t,x) &:= \sum_{j=1}^{n} \rho_j(t)\, \psi_j(x), \\
\phi(t,x) \sim \phi^{(n)}(t,x) &:= \sum_{j=1}^{n} \phi_j(t)\, \psi_j(x), \\
\mu(t,x) \sim \mu^{(n)}(t,x) &:= \sum_{j=1}^{n} \mu_j(t)\, \psi_j(x), \\
U(t,x) \sim u^{(n)}(t,x) &:= \sum_{j=1}^{n} V_j(t)\, \chi_j(x).
\end{aligned}
$$

Proof

- Galerkin–approximation in space $\Rightarrow$ system

$$\boxed{M(\phi_h, \rho_h)x_h = f_h(\phi_h, \rho_h)}$$

for $x_h = (v_h, \mu_h, \partial_t \phi_h, \partial_t \rho_h, U_h)^\top$

- M is regular: Proof similar to energy estimate
- Transformation to system

$$\boxed{\partial_t \begin{pmatrix} \phi_h \\ \rho_h \end{pmatrix} = F \begin{pmatrix} \phi_h \\ \rho_h \end{pmatrix}}$$

with Lipschitz function F
$\Rightarrow$ existence of discrete solution local in time

- Energy estimate:

$$\boxed{\begin{aligned}&\|\rho_h\|_{L_\infty(I;L_2(\Omega))} + \|\phi_h\|_{L_\infty(I;L_2(\Omega))} + \|U_h\|_{L_\infty(I;H^1(\Omega))}\\ &+ \|\boldsymbol{v}_h\|_{L_2(I;H^1(\Omega))} + \left\|\sqrt{K(\phi_h)}\nabla\rho_h\right\|_{L_2(I\times\Omega)}\\ &+ \|\nabla\mu_h\|_{L_2(I\times\Omega)} + \|\partial_t\phi_h\|_{L_2(I\times\Gamma)} \leq c\end{aligned}}$$

  Estimate for partial time derivative

$$\boxed{\|\rho_h\|_{H^\nu(I;L_2(\Omega))} + \|\phi_h\|_{H^\nu(I;L_2(\Omega))} \leq C(\nu)}$$

  with $\nu \in (0, 1/2)$

- For nondegenerate K:
  Subsequence converges to solution of problem

The convective terms give cubic contributions to the integral

$$\int_\Omega \left(\partial_t \rho\, \psi + \boxed{v \cdot \nabla \rho\, \psi} + K(\phi)\nabla(V + \lambda\rho)\nabla\psi\right) dx = \int_\Omega q\, \psi\, dx,$$

$$\int_\Omega \left(\partial_t \phi\, \psi + \boxed{v \cdot \nabla \phi\, \psi} + M(\phi)\nabla\mu \cdot \nabla\psi\right) dx = 0,$$

By compensated compactness

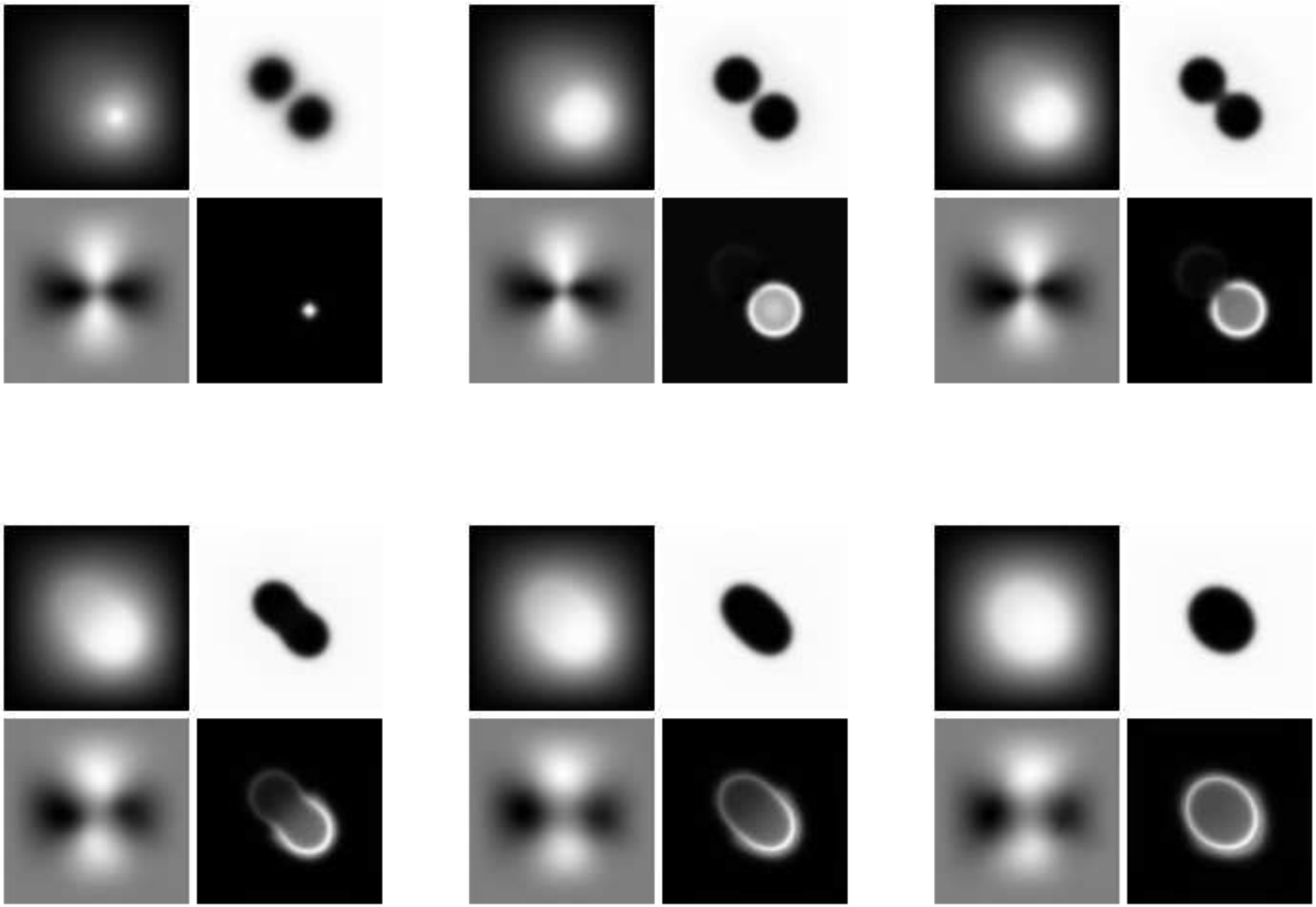
$$v^{(n)} \cdot \nabla \rho^{(n)} \rightharpoonup v \cdot \nabla \rho \ \text{ and } \ v^{(n)} \cdot \nabla \phi^{(n)} \rightharpoonup v \cdot \nabla \phi \ \text{ in } L_1(I \times \Omega),$$

The case of degenerate K

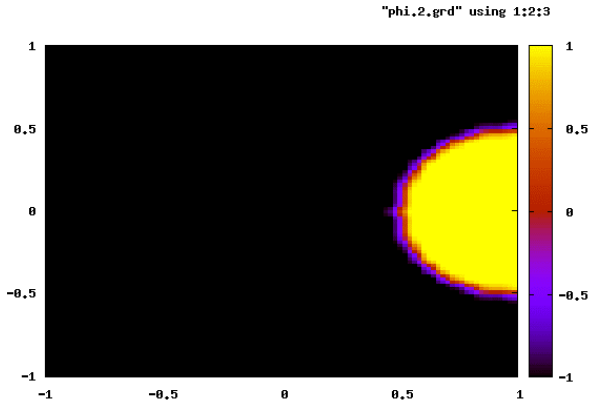
Problem: Convergence $K(\phi_h)\nabla\rho_h \rightharpoonup K(\phi)\nabla\rho$

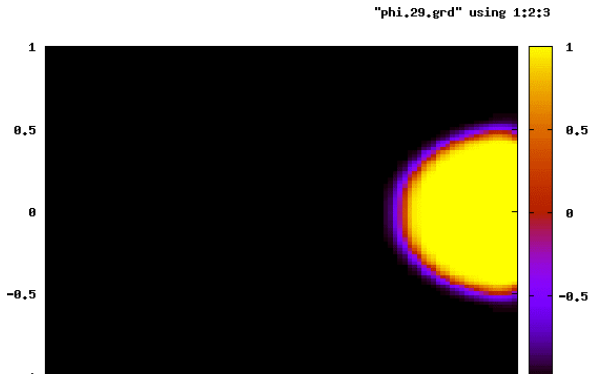
- Approximation with nondegenerate $K(\phi)+\eta$
  Existence of solution $(\boldsymbol{v}_\eta, \phi_\eta, \mu_\eta, \rho_\eta, U_\eta)$
- Regularity $\phi \in L_2(I; H^\beta(\Omega))$ with $1 < \beta < 3/2$
  for continuous $\varepsilon(\phi)$
- Convergence $\eta \to 0$
  strong convergence of $\nabla\phi_\eta \to \nabla\phi$ in $L_2(I \times \Omega)$

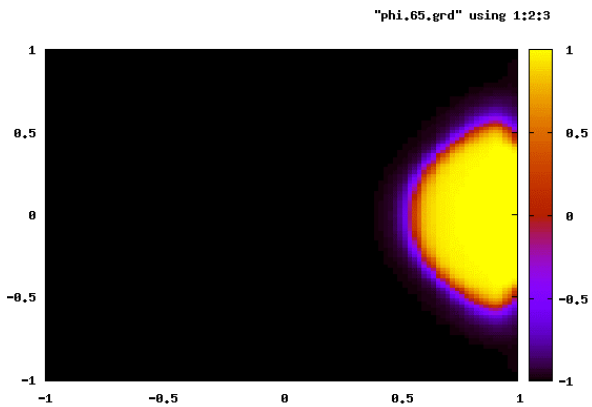
Preliminary numerical tests (2D)



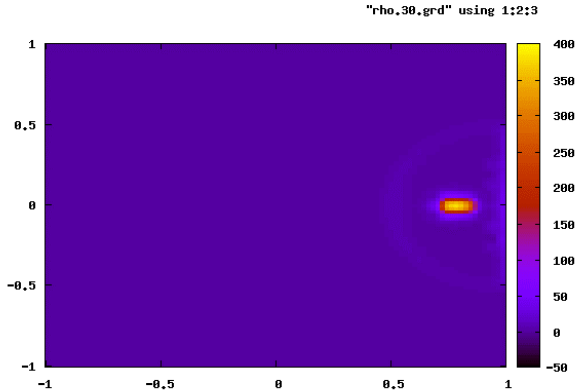
Phase field

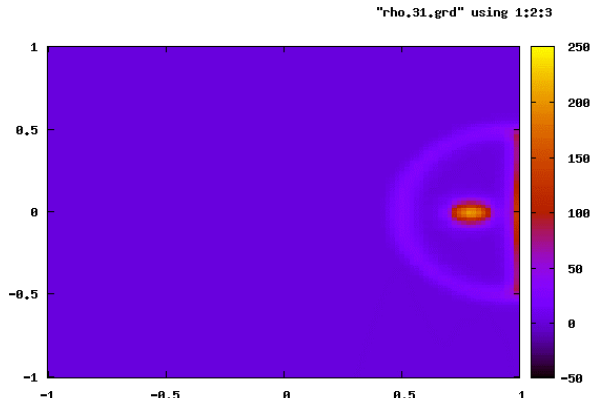


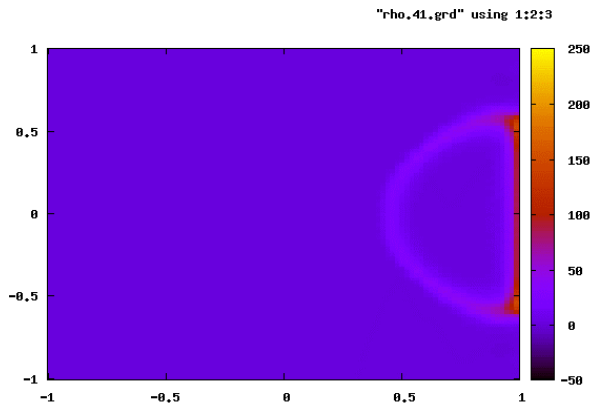




Charge density







Still to be done

- Numerical implementation (in progress)
- Condition for potential instead of charge source
- Non–degenerate $K(\phi)$ & non–constant $\varepsilon(\phi)$
- Regularity, uniqueness
- Model with Navier–condition for velocity
- Modify Ohm's law for electrolites:

$$\boldsymbol{J_D} = K(\phi)(\rho \boldsymbol{E} - \lambda \nabla \rho)$$