

# A mathematical point of view in Electrowetting

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*In collaboration with*

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and Patrick Ciarlet Jr. (ENSTA, Paris, France).*

6<sup>th</sup> singular days

30 April 2010

# Electrowetting

# Wetting?



Hydrophobic →



← Hydrophilic

# Wetting?



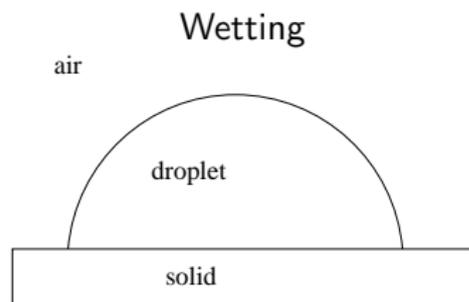
Hydrophobic →



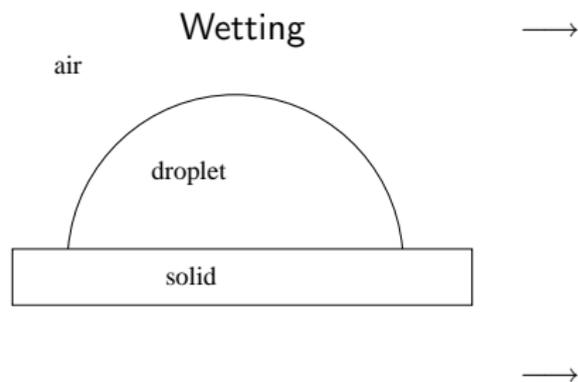
← Hydrophilic

How to control wetting?

# What is Electrowetting?

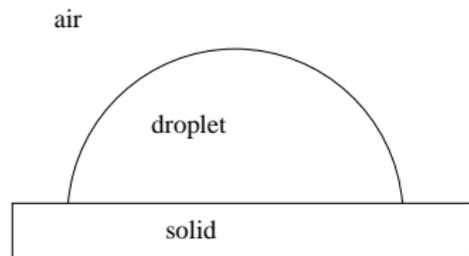


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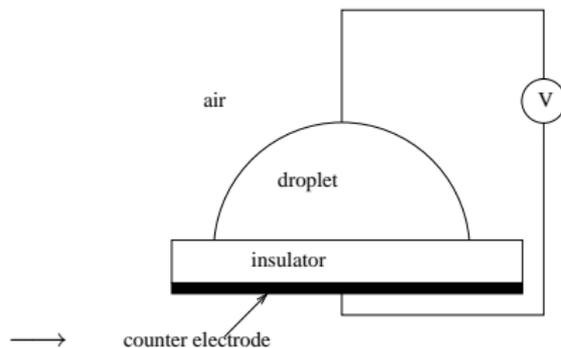


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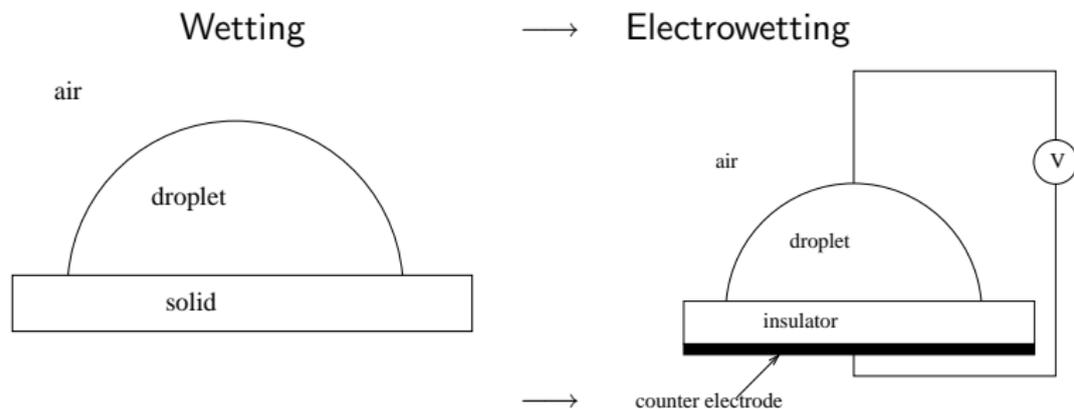
Wetting



→ Electrowetting

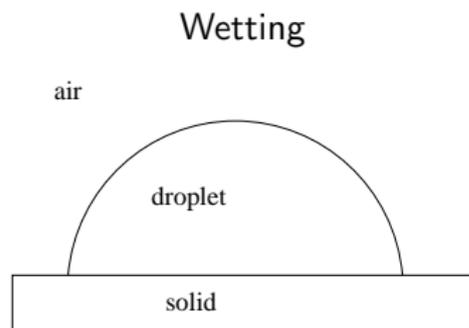


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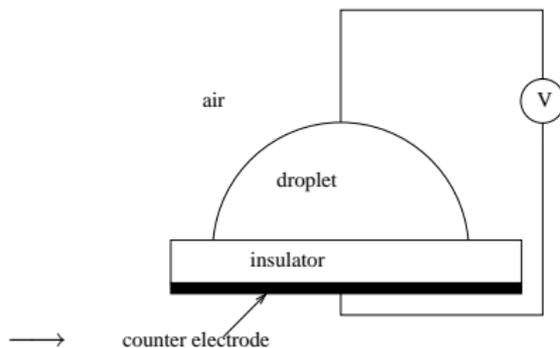


Modify the **affinity** between solid and liquid

# What is Electrowetting?



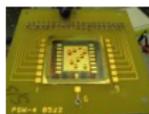
→ Electrowetting



→ Due to **Bruno Berge** : 1993

*Many applications :*

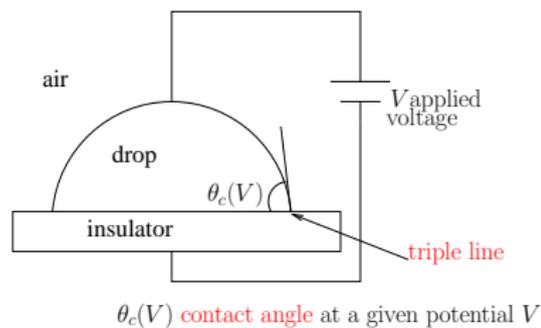
- Variable focal liquid lenses
- Microfluidics



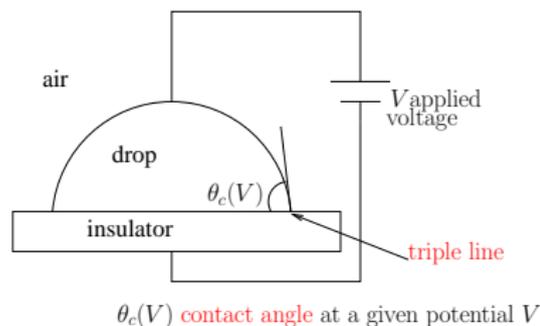
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- 1 Introduction
- 2 Modelling Electrowetting
- 3 Numerical results in the axisymmetric case
- 4 Numerical study of the 3D case
  - Stakes
  - Numerical approximation
- 5 Conclusion and further works

# Observations and approximations

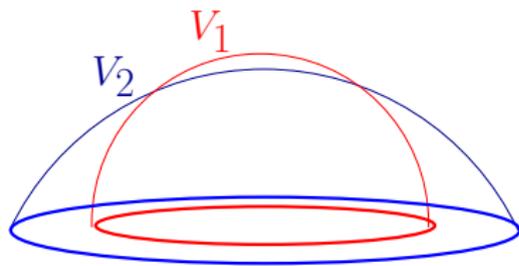
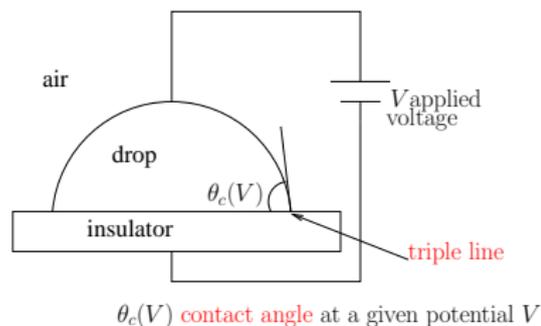


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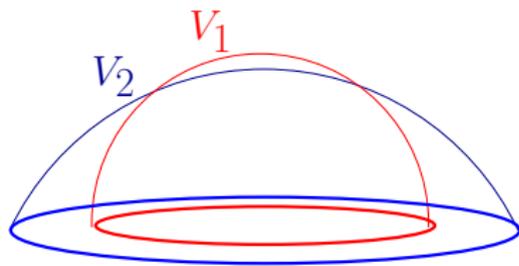
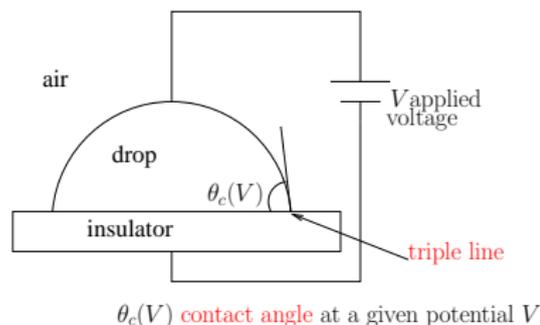
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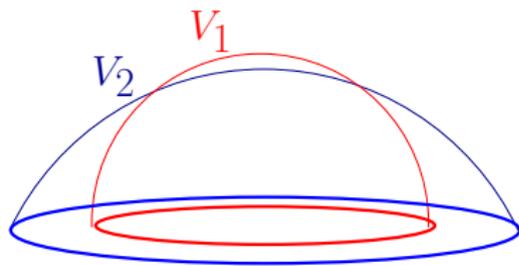
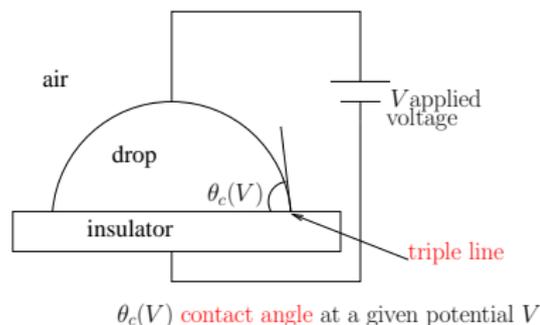
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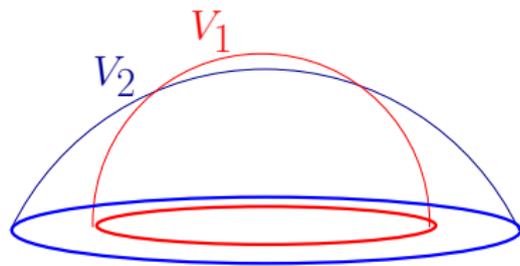
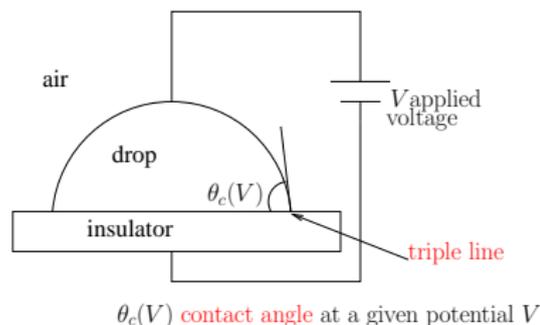
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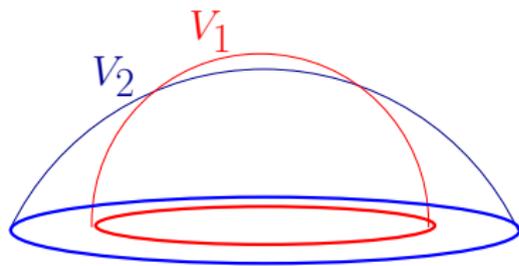
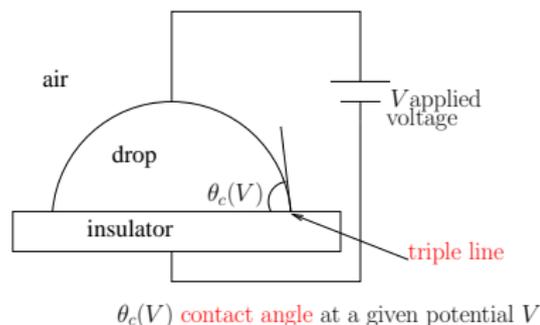
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  - Physical predictions  $\theta_c = \theta_Y$  for all  $V$ !

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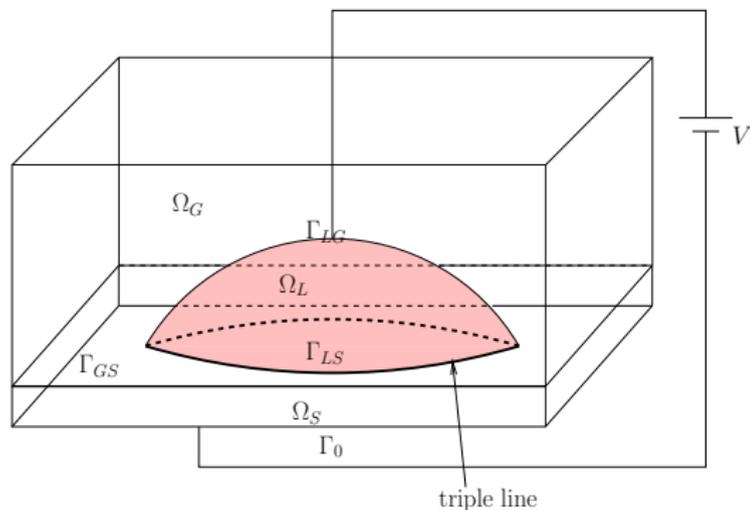
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What can we add as mathematicians?

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# Notations



$$\Omega = \Omega_G \cup \Omega_S \cup \Gamma_{GS}, \text{ (white domain)}$$

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 $\varepsilon$  : permittivity ( $\varepsilon = \varepsilon_G$  in  $\Omega_G$ ,  $\varepsilon = \varepsilon_S$  in  $\Omega_S$ )
- $J(\Omega) := \mathcal{E}(\Omega_L, V) = J_{grav}(\Omega) + J_{LS}(\Omega) + J_{LG}(\Omega) + J_{elec}(\Omega)$   
**cost function** of the problem.

# The potential: transmission problem

$$\left\{ \begin{array}{ll} \operatorname{div}(\varepsilon_i \nabla \phi^\Omega) = 0 & \text{in } \Omega_i \quad i = G, S \\ \phi^\Omega = V & \text{on } \Gamma_{LG} \cup \Gamma_{LS} \\ \phi^\Omega = 0 & \text{on } \Gamma_0 \\ \phi_G^\Omega = \phi_S^\Omega & \text{on } \Gamma_{GS} \\ \varepsilon_G \nabla \phi_G^\Omega \cdot \vec{N}_G = -\varepsilon_S \nabla \phi_S^\Omega \cdot \vec{N}_S & \text{on } \Gamma_{GS} \\ \varepsilon_i \nabla \phi_i^\Omega \cdot \vec{N}_i = 0 & i = G, S \text{ on artificial boundaries} \end{array} \right.$$

- $\phi^\Omega$  depends on  $\Omega$ .
- $\Omega$  has a **reentrant corner** due to the triple line  $\Rightarrow$  **Loss of regularity**

# Optimal shape

To  $V \geq 0$  and a given volume  $vol$ ,

$$(P) \left\{ \begin{array}{l} \text{Find } \Omega_L^* \text{ such that:} \\ \mathcal{E}(\Omega_L^*, V) = \min_{\{\Omega_L; \text{Vol}(\Omega_L)=vol\}} \mathcal{E}(\Omega_L, V) \end{array} \right.$$

- *Optimization under constraint* treated by a Lagrangian  $\mathcal{L}(\Omega, \lambda) = J(\Omega) - \lambda C(\Omega)$ , where  $C(\Omega) = \text{Vol}(\Omega_L) - vol$ ,  $\lambda \in \mathbb{R}$ .
- **Shape optimization** gives a necessary condition for optimality:

$$\forall U \in \mathcal{U} \subset \mathcal{C}^1(\Omega^*, \mathbb{R}^3), DJ(\Omega^*).U = \lambda^* DC(\Omega^*).U$$

if  $\Omega^*$  saddle point and where  $DJ(\Omega^*)$  is the shape derivative of  $J$  in  $\Omega^*$ .

- Using the **expression of the singularity at the triple line** one obtains

The contact angle  $\theta_c$  is independent of the applied potential  $V \geq 0$  i.e.

$$\theta_c(V) = \theta_Y, \forall V \geq 0$$

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# Numerical approximation : axisymmetric case

$V$  and physical constants are given.

Computation of the numerical shape, curvature and contact angle of the saddle point.

## Difficulties arise at the triple point

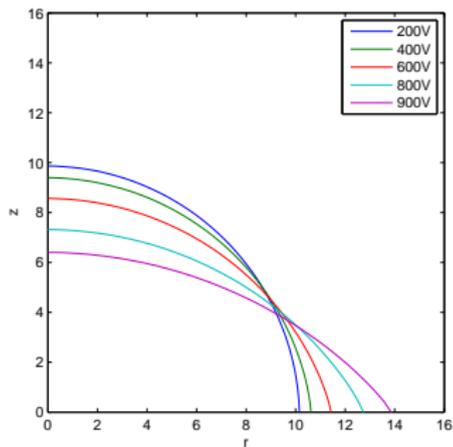
- Need to adopt a microscopic view of the model at the triple point:  
→ "Macro-Micro" coupling model.
- Need to compute accurately the potential close to the triple point:  
→ Use of the Singular Complement Method (Ciarlet Jr. and al).

# Numerical approximation : axisymmetric case

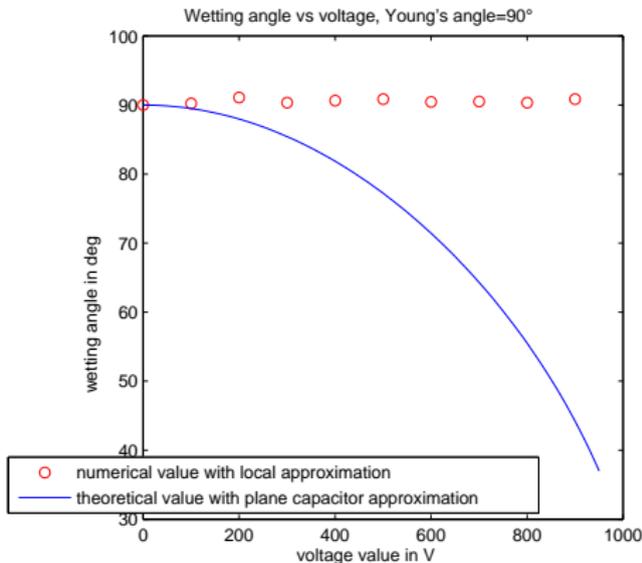
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### Shape of the drop



### Contact angle



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## 3D case: stakes

- Need of a good approximation of the **electrostatic field** and of **its trace on the boundary of the drop**
- Singular Complement Method less efficient in 3D than in 2D.

### *Method:*

- **Computation of the field**, instead of the potential.
- **Weighted weak formulation** on the divergence of the field in order to solve the problem induced by the singularity (M. Costabel, M. Dauge, *Numer. Math.* 2002; P. Ciarlet Jr. et al., *M2AN*).

### *Point of view adopted:*

- **Numerical Analysis** instead of computations.

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## Field formulation and space considered

The field  $E^\Omega$  is solution of:

$$\left\{ \begin{array}{ll} \operatorname{curl} E_i^\Omega = 0 & \text{in } \Omega_i \quad i = G, S \\ \operatorname{div}(\varepsilon_i E_i^\Omega) = 0 & \text{in } \Omega_i \quad i = G, S \\ E_i^\Omega \times n = 0 & \text{on } \Gamma_{LG} \cup \Gamma_{LS} \cup \Gamma_0 \\ \varepsilon_G E_G^\Omega \cdot n = \varepsilon_S E_S^\Omega \cdot n, \quad E_G^\Omega \times n = E_S^\Omega \times n & \text{on } \Gamma_{GS} \\ \varepsilon E^\Omega \cdot n = 0 & \text{on the artificial boundaries} \end{array} \right.$$

- Space considered: For  $\alpha \in ]0, 1[$ ,

$$\mathcal{X}_\alpha := \{ \mathcal{F} \in H(\operatorname{curl}, \Omega) \mid w_\alpha \operatorname{div} \varepsilon \mathcal{F} \in L^2(\Omega), \quad \mathcal{F} \times n|_{\Gamma_0 \cup \Gamma_L} = 0, \quad \varepsilon \mathcal{F} \cdot n|_{\Gamma_{\text{ext}}} = 0 \}$$

where  $w_\alpha(\cdot) \approx \operatorname{dist}(\cdot, \text{triple ligne})^\alpha$ .

- The boundary of  $\Omega$  has two connected components.  
For  $\alpha \in ]0, 1[$ ,

$$\|\mathcal{F}\|_{\mathcal{X}_\alpha} := \left( \|\operatorname{curl} \mathcal{F}\|_{L^2}^2 + \|w_\alpha \operatorname{div}(\varepsilon \mathcal{F})\|_{L^2}^2 + \left| \int_{\Gamma_0} \varepsilon \mathcal{F} \cdot n \right|^2 \right)^{\frac{1}{2}}$$

is an equivalent norm to the graph norm.

- $E^\Omega$  is **completely characterized** if one adds the equation:

$$\int_{\Gamma_0} \varepsilon E^\Omega \cdot n d\Gamma = -\mathbb{C}V$$

where  $\mathbb{C} = \int_{\Omega} \varepsilon \nabla \chi_0^\Omega \cdot \nabla \chi_0^\Omega d\Omega$  is the capacitance matrix, with

$$\begin{cases} \operatorname{div}(\varepsilon \nabla \chi_0^\Omega) = 0 & \text{in } \Omega_i \quad i = G, S \\ \chi_0^\Omega = 0 & \text{on } \Gamma_{LG} \cup \Gamma_{LS} \\ \chi_0^\Omega = 1 & \text{on } \Gamma_0 \\ + \text{Transmission conditions} \end{cases}$$

- Denote

$$PH^1(\Omega) := \{v \in L^2(\Omega) \mid v \in H^1(\Omega_G) \text{ and } v \in H^1(\Omega_S)\}$$

There exists  $\alpha_{min} \in ]0, 1[$  such that

$$\mathcal{X}_\alpha \cap (PH^1(\Omega))^3 \text{ is dense in } \mathcal{X}_\alpha \text{ for all } \alpha \in ]\alpha_{min}, 1[$$

$\Rightarrow$  Approximation by Lagrange Finite Elements envisageable.

# Weak formulation and numerical approximation

*Continuous weak formulation*

$$a(E^\Omega, \mathcal{F}) = l(\mathcal{F}), \quad \forall \mathcal{F} \in \mathcal{X}_\alpha$$

$$a(\mathcal{E}, \mathcal{F}) := \int_{\Omega} \operatorname{curl} \mathcal{E} \cdot \operatorname{curl} \mathcal{F} d\Omega + \sum_{i=G,S} \varepsilon_i^{-2} \int_{\Omega_i} w_\alpha \operatorname{div}(\varepsilon \mathcal{E}) w_\alpha \operatorname{div}(\varepsilon \mathcal{F}) d\Omega + \varepsilon_S^{-2} \int_{\Gamma_0} \varepsilon \mathcal{E} \cdot n \int_{\Gamma_0} \varepsilon \mathcal{F} \cdot n \quad (1)$$

and  $l(\mathcal{F}) = -\mathbb{C}V \int_{\Gamma_0} \varepsilon \mathcal{F} \cdot n$ .

# Weak formulation and numerical approximation

*Continuous weak formulation*

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and  $l(\mathcal{F}) = -\mathbb{C}V \int_{\Gamma_0} \varepsilon \mathcal{F} \cdot n$ .

*Approximation*

$\mathcal{T}_h$  family of meshes of  $\Omega$ .

$E_h^\Omega \in \mathcal{X}_{h,k} := \{ \mathcal{F}_h \in \mathcal{X}_\alpha \cap (PH^1(\Omega))^3 \mid (\mathcal{F}_h)_{K_l} \in (\mathbb{P}_k(K_l))^3, \quad \forall K_l \in \mathcal{T}_h \}$  solution of

$$a(E_h^\Omega, \mathcal{F}_h) = l_h(\mathcal{F}_h), \quad \forall \mathcal{F}_h \in \mathcal{X}_{h,k}$$

where  $l_h$  is an approximation of  $l$ .

- In our particular case, we know the value of  $\alpha_{min}$  :

$$\alpha_{min} = 1 - \min \nu_Y(s),$$

and  $\nu_Y(s)$  is the unique solution in  $]0, 1[$  of the equation:

$$\varepsilon_S \tan(\nu_Y(s)(\pi - \theta_Y(s))) = -\varepsilon_G \tan(\nu_Y(s)\pi).$$

- Error estimation obtained:

$$\forall \eta > 0, \quad \exists C_\eta, \quad \|E^\Omega - E_h^\Omega\|_{\mathcal{X}_\alpha} \leq C_\eta h^{\alpha - \alpha_{min} - \eta}$$

- Normal trace defined in  $H^{-\frac{1}{2}}(\partial\Omega)$  and:

$$\forall \eta > 0, \quad \exists C_\eta, \quad \|\varepsilon E^\Omega \cdot n - \varepsilon E_h^\Omega \cdot n\|_{H^{-\frac{1}{2}}(\partial\Omega)} \leq C_\eta h^{\alpha - \alpha_{min} - \eta}$$

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# Conclusions

- Modelling of Electrowetting phenomena
- Numerical simulation in the axisymmetric case.
- Numerical Analysis in 3D.

Taking into account the singularity is essential!!

## Further works

- Saturation of the contact angle: Something is missing in the model!  
Corona discharge phenomenon.
- Non static case: Singularity to be taken into account.
- Existence of the optimal shape...
- Computations in the 3D case.