Equivalent electrostatic capacitance Computation using FreeFEM++

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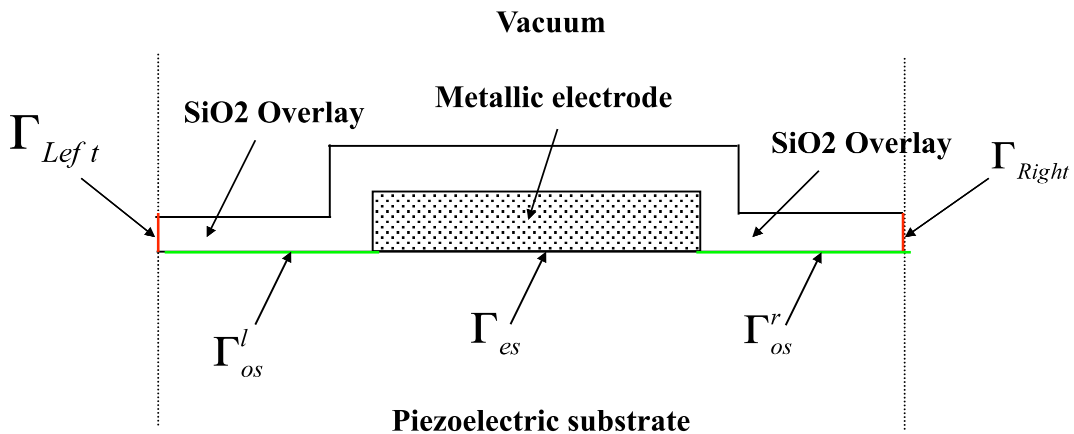
Outlines

- **Physical model**
- **The Electrostatic Computation : FreeFem++ Model**
- **Validations**
- **Conclusions**

Physical model

- Geometry :



- Assumptions :
  - 2D analysis (very long electrode) : Plain strain approximation
  - Semi-infinite piezoelectric medium
  - Electrical assumption : the upper half space behaves like an homogenous dielectric medium
  - Mechanical assumption : the metallic electrode and the SiO_2 overlay are homogeneous isotropic, elastic materials
  - Electrical charge distribution : interface electrode / substrate

Physical Model

Semi-infinite piezoelectric substrate

Integral formulation with harmonic periodic boundary conditions

Mechanical displacement

Mechanical stress vector

Semi-infinite homogeneous Green's function

$$\begin{pmatrix} \mathbf{u}(x) \\ \phi(x) \end{pmatrix} = \int_{-p/2}^{+p/2} \mathbf{G}_\gamma^p (x - x') \begin{pmatrix} \mathbf{t}_s(x') \\ \Delta d_2(x') \end{pmatrix} dx' \qquad \mathbf{G}_\gamma^p(x) = \sum_{n=-\infty}^{+\infty} \mathbf{G}(x - np) e^{-j2\pi n\gamma}$$

Electric displacement

Periodic Harmonic Green's function

Jump in the normal electric displacement

Physical Model

Electrode and Overlay (mechanical behavior)

- The Variational Formulation for the elastic problem : finding **u** satisfying whatever the virtual displacement **v** :

Stress tensor — displacement field — Strain tensor — virtual displacement field

$$\int_{\Omega_e} \mathbf{T}(\mathbf{u}):\mathbf{S}(\mathbf{v})\,d\Omega + \int_{\Omega_{ov}} \mathbf{T}(\mathbf{u}):\mathbf{S}(\mathbf{v})\,d\Omega - \rho_e\omega^2\int_{\Omega_e} \mathbf{u}.\mathbf{v}\,d\Omega - \rho_{ov}\omega^2\int_{\Omega_{ov}} \mathbf{u}.\mathbf{v}\,d\Omega$$

$$= \int_{\Gamma_{es/os}} \mathbf{t}_s.\mathbf{v}\,d\Gamma + \int_{\Gamma_{Left}} \mathbf{t}_s.\mathbf{v}\,d\Gamma + \int_{\Gamma_{Right}} \mathbf{t}_s.\mathbf{v}\,d\Gamma$$

Stress vector

- Periodic harmonic boundary conditions :

$$\begin{cases} \mathrm{u}(-p/2, y) = e^{-j2\pi\gamma}\,\mathrm{u}(p/2, y) \\ \mathrm{t}_s(-p/2, y) = -e^{-j2\pi\gamma}\,\mathrm{t}_s(p/2, y) \end{cases}, \quad \text{for } y \in \Gamma_{Right}$$

Physical Model

Homogeneous dielectric constant (upper half space)

- Electrostatic computation of the harmonic capacitance using the finite element tool Freefem++ (the piezoelectric substrate, the electrode and the overlay are assumed dielectric media)

- The analytical expression of the harmonic capacitance of a single periodic array of electrodes with negligible thickness is used :

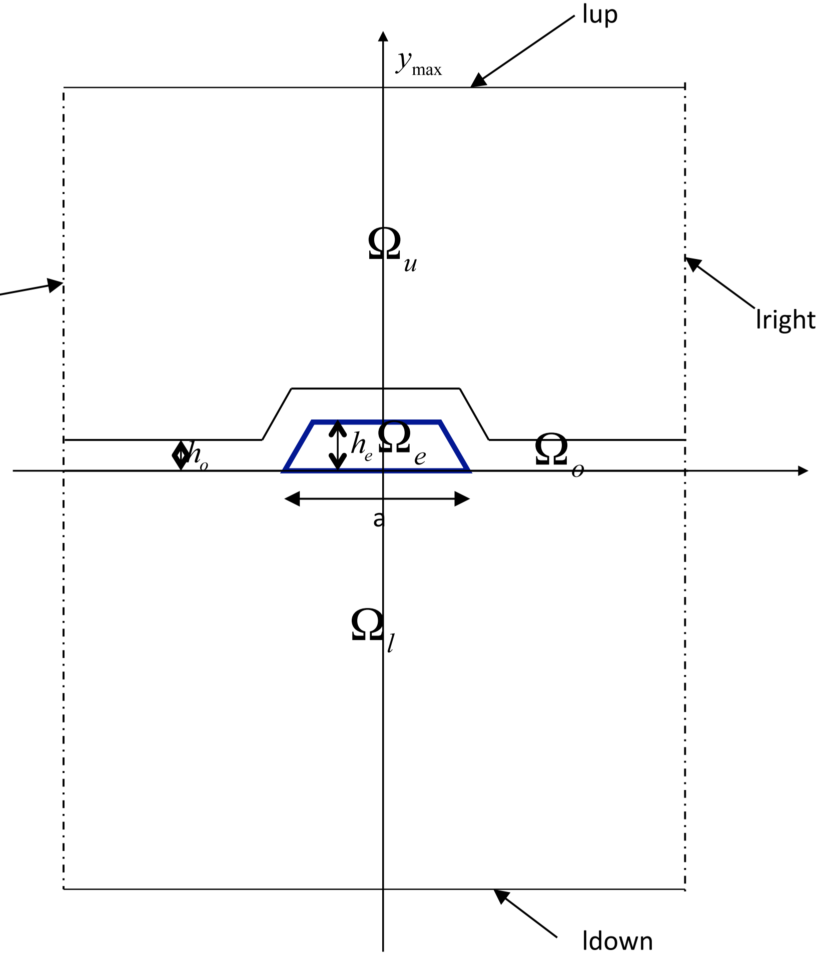
Legendre's function of the first kind

$$C(\gamma) = 2\left(\varepsilon_0 + \varepsilon_u^{eq}\right)\sin(\pi\gamma)\frac{\mathrm{P}_{-\gamma}\left(\cos(\pi\, a/p)\right)}{\mathrm{P}_{-\gamma}\left(-\cos(\pi\, a/p)\right)}$$

effective permittivity of the upper half space

effective permittivity of the substrate

FreeFem++ Model



Schematic of the electrostatic problem

FreeFem++ Model

- The quasi static Maxwell's equation is verified for the regions Ω_u Ω_o Ω_l

$$\begin{cases} D = \varepsilon_{u,l,o} E \\ E = -\nabla \phi \end{cases}$$

- No surface charge density at the up and low interfaces

FreeFem++ Model

- The Variational Formulation : Finding the potential Φ defined in Ω, verifying whatever the test potential function defined also in Ω

$$-\int_{\Omega_u} \varepsilon_u \mathrm{E}(\Phi) \bullet \mathrm{E}(\varphi) d\Omega - \int_{\Omega_o} \varepsilon_o \mathrm{E}(\Phi) \bullet \mathrm{E}(\varphi) d\Omega - \int_{\Omega_l} \varepsilon_l \mathrm{E}(\Phi) \bullet \mathrm{E}(\varphi) d\Omega$$

$$= \int_{\Gamma_{el} \cup \Gamma_{eo}} \left(\mathrm{D}(\Phi) \bullet \mathrm{n} \right) \varphi d\Gamma$$

FreeFem++ Model

- Finally the periodic harmonic boundary conditions relating the left and right interfaces have been taken into account using Lagrange Multipliers.

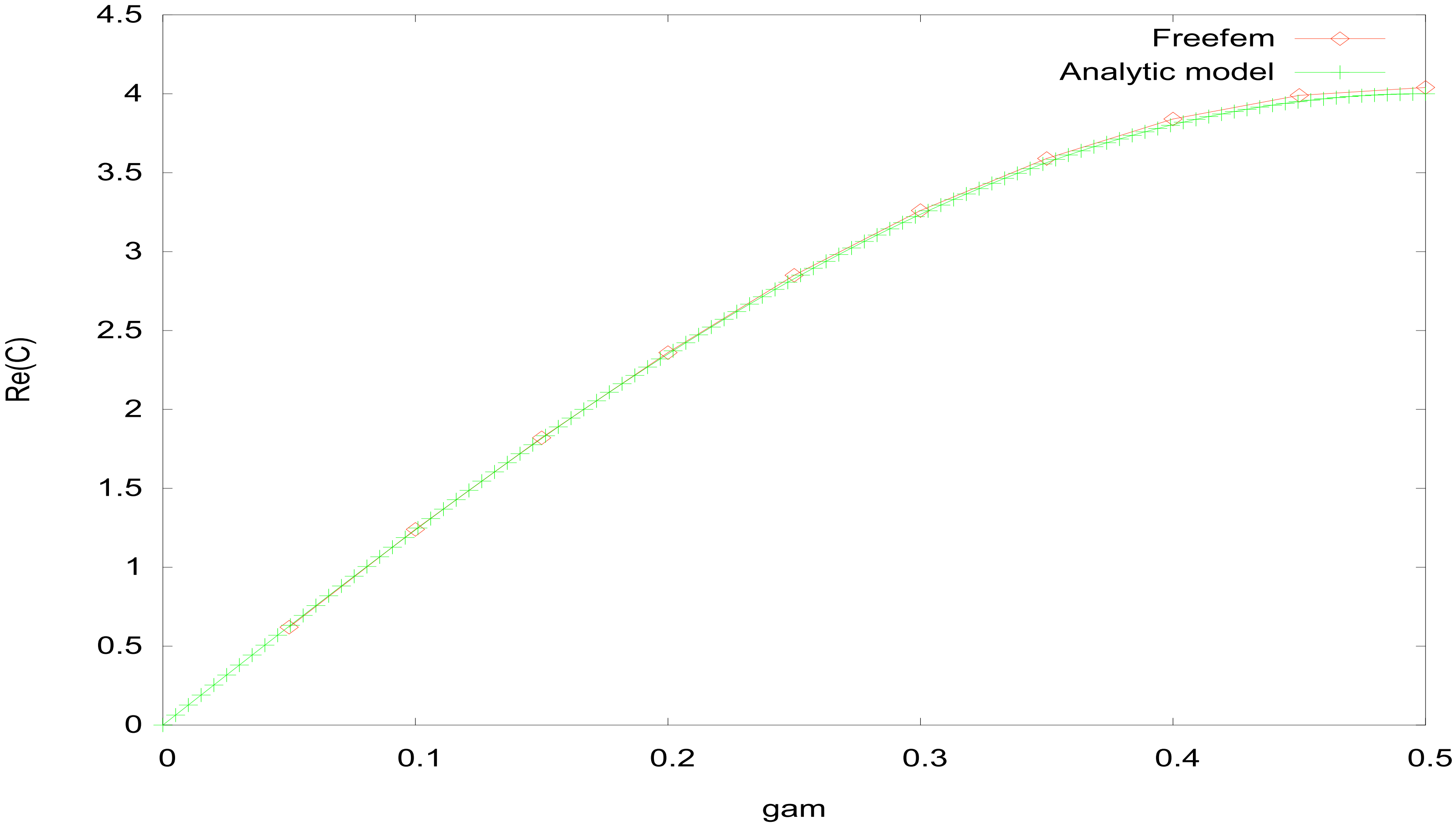
$$\Phi_{\Gamma_l}\left(+p/2\,,y\right) = \Phi_{\Gamma_r}\left(-p/2\,,y\right)\exp\left(-j2\pi\gamma\right)$$

P periodic functions

$$\int_{\Gamma_l}\left(\Phi\left(M\right) - \exp\left(j2\pi\gamma\right)\Phi\left(P_{rl}\left(M\right)\right)\right)\varphi d\Gamma = 0$$

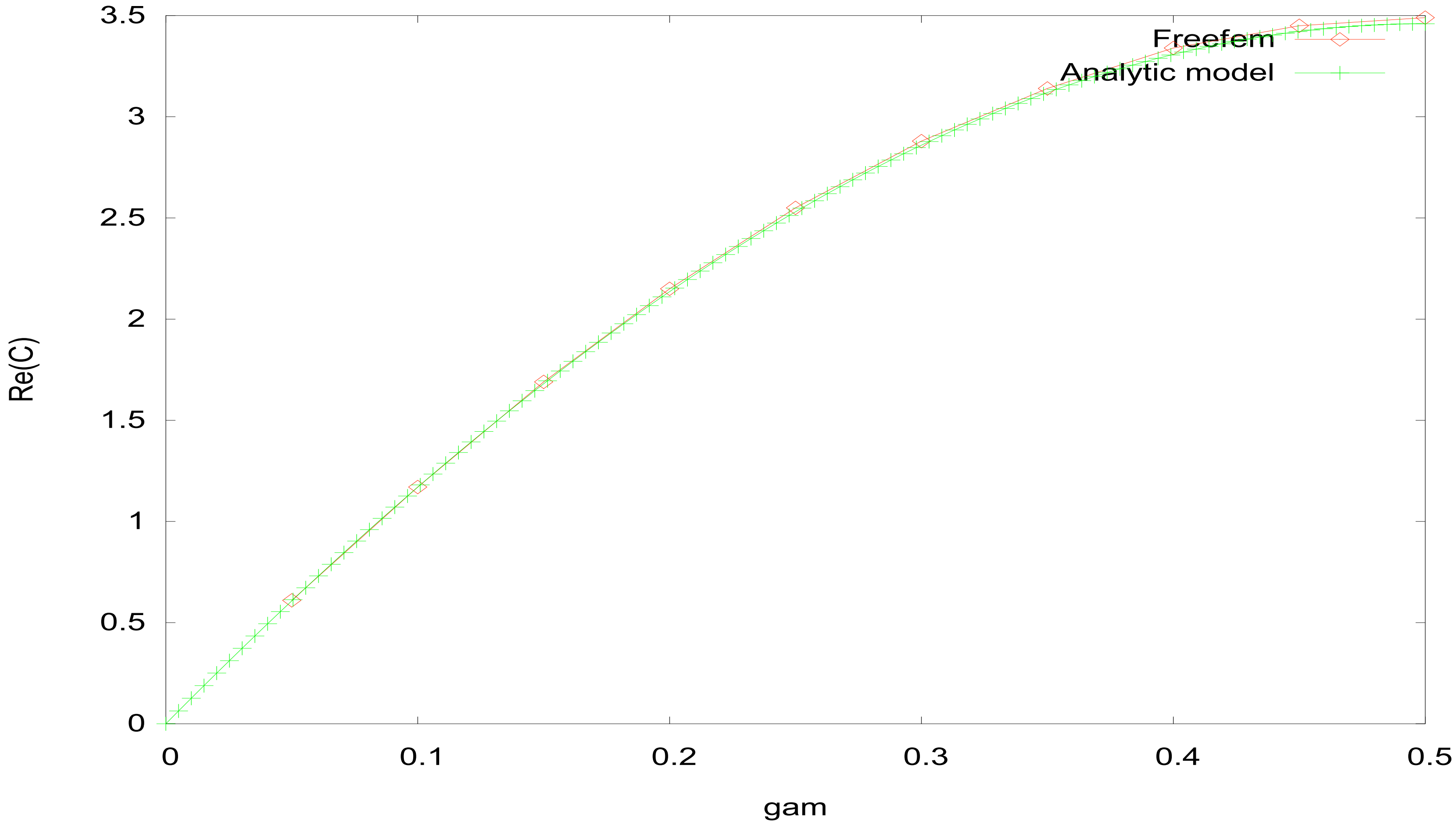
Projection from Left to Right

FreeFem++ Model



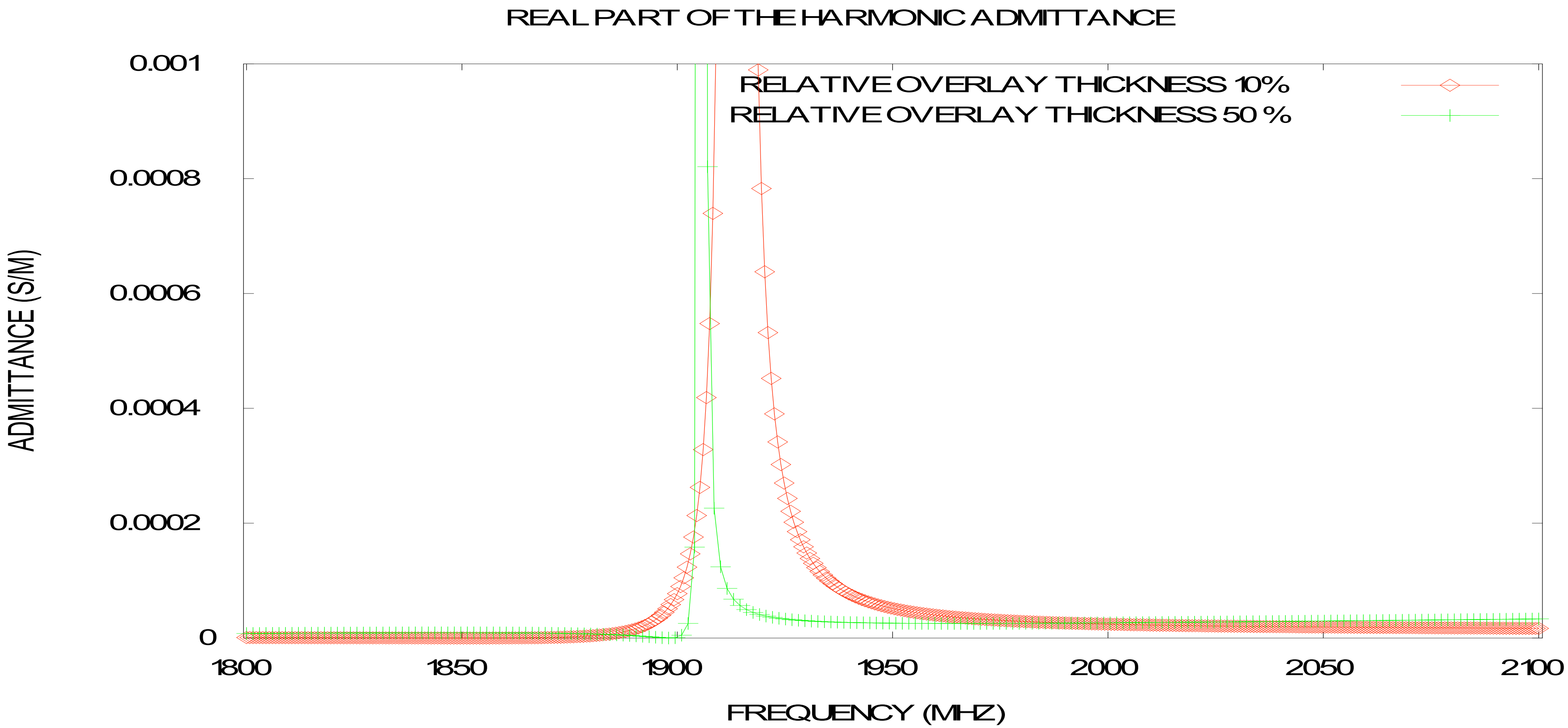
Capacitance of uniform array in vacuum (a/p=0.5), (red : FreeFem, green : analytical computation)

FreeFem++ Model



Capacitance of uniform array in vacuum (a/p=0.4), (red : FreeFem, green : analytical computation)

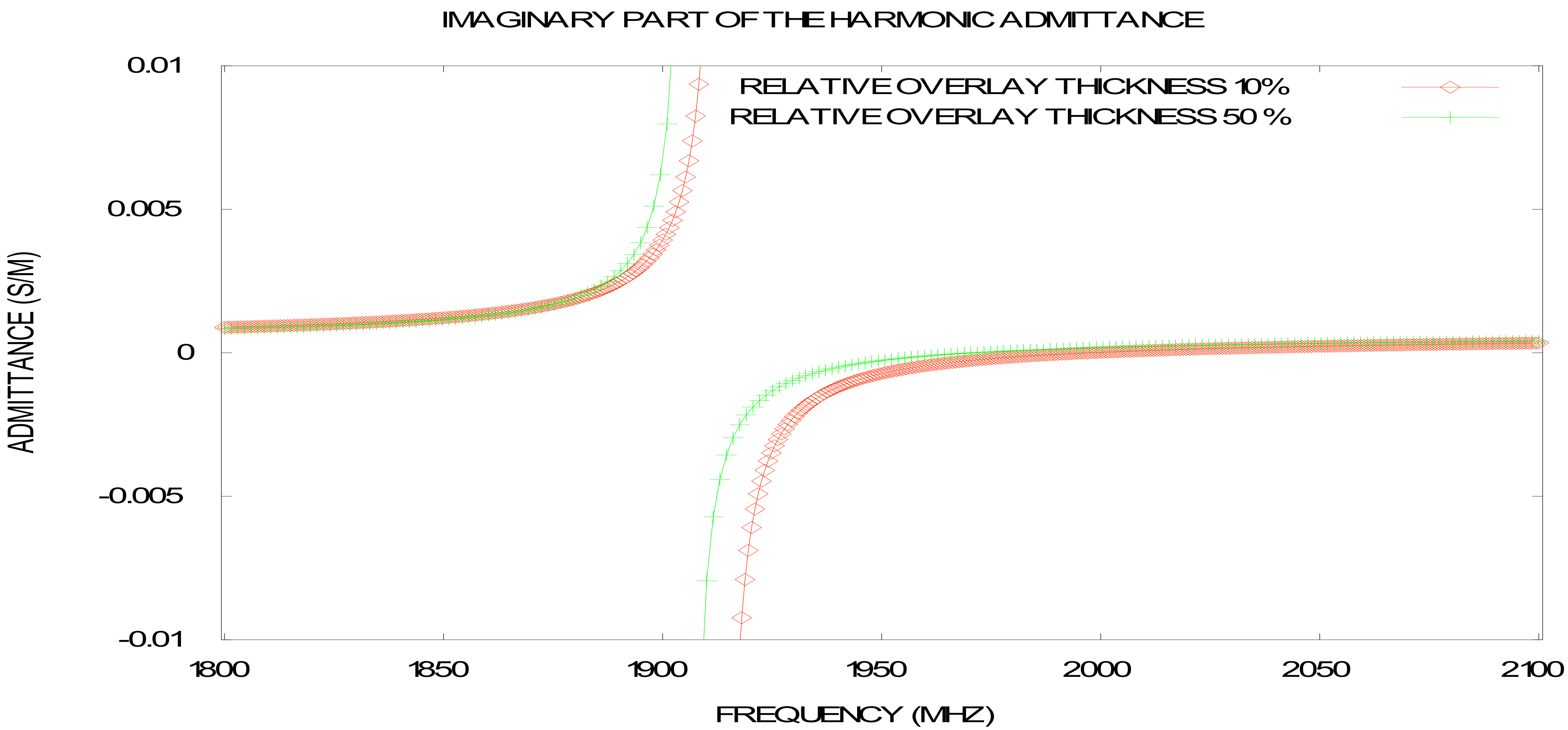
Harmonic admittance computations



Copper metallic electrodes covered with an SiO_2 overlay

The piezoelectric substrate is YX+36° $LiTaO_3$

Harmonic admittance computations



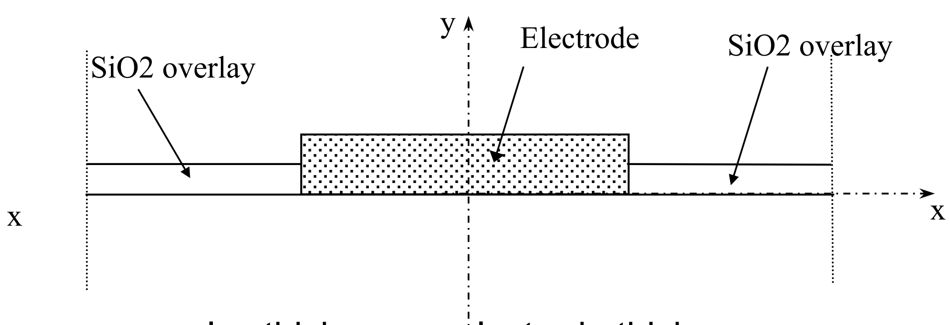
Copper metallic electrodes covered with an SiO_2 overlay

The piezoelectric substrate is YX+36° $LiTaO_3$

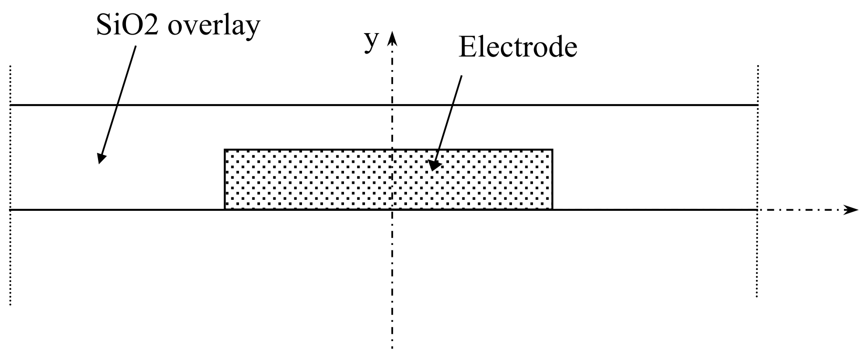
Software validations

The geometry of the problem

- Asumptions :
  - Rectangular Copper Electrodes (0.5 line ratio)
  - SiO_2 Overlay
  - The piezoelectric cut is YX+36° $LiTaO_3$
  - Homogenous effective dielectric permittivity for the upper half space 1



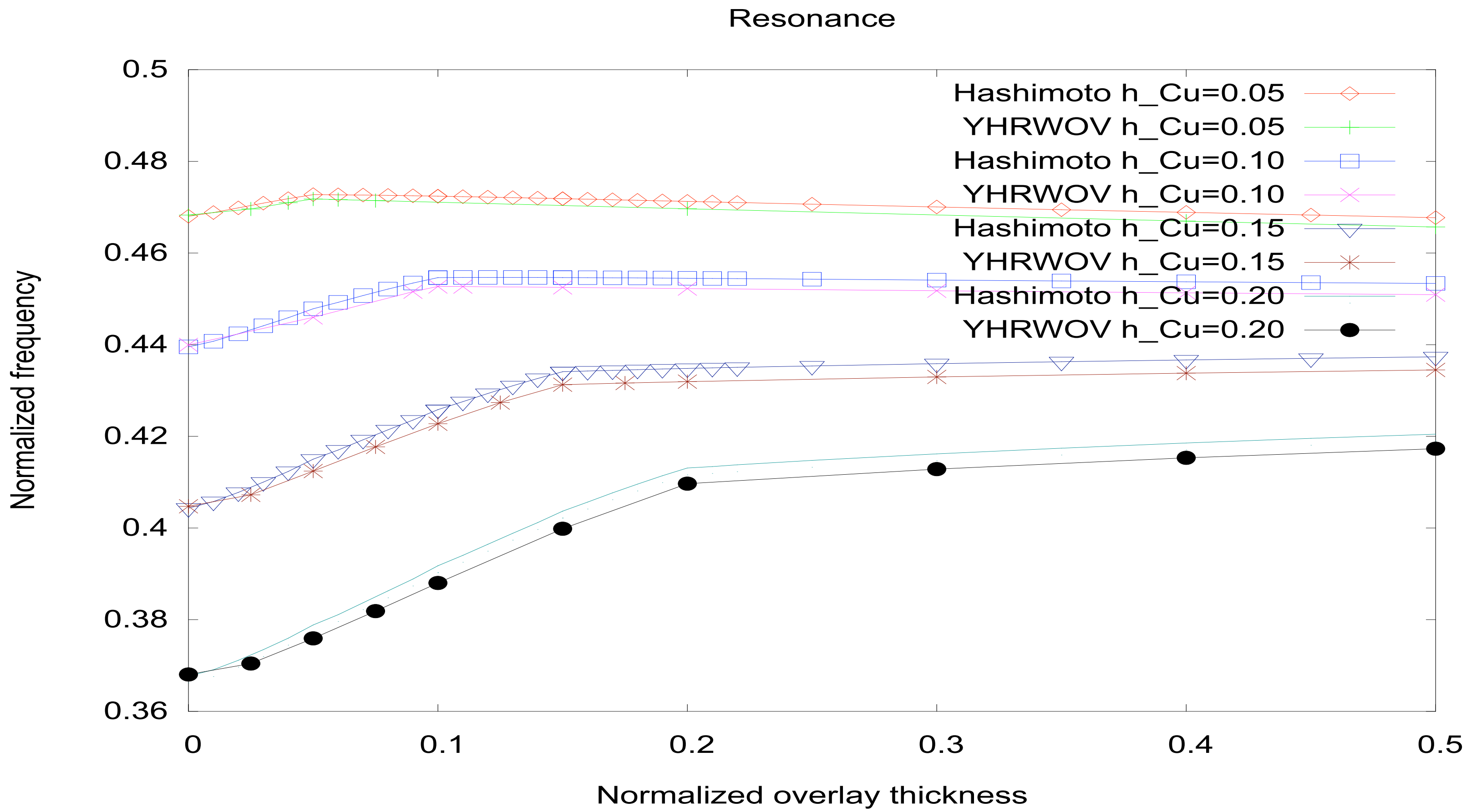
overlay thickness < electrode thickness



overlay thickness > electrode thickness

Software validations

Comparison with K. Hashimoto’s data



Software validations

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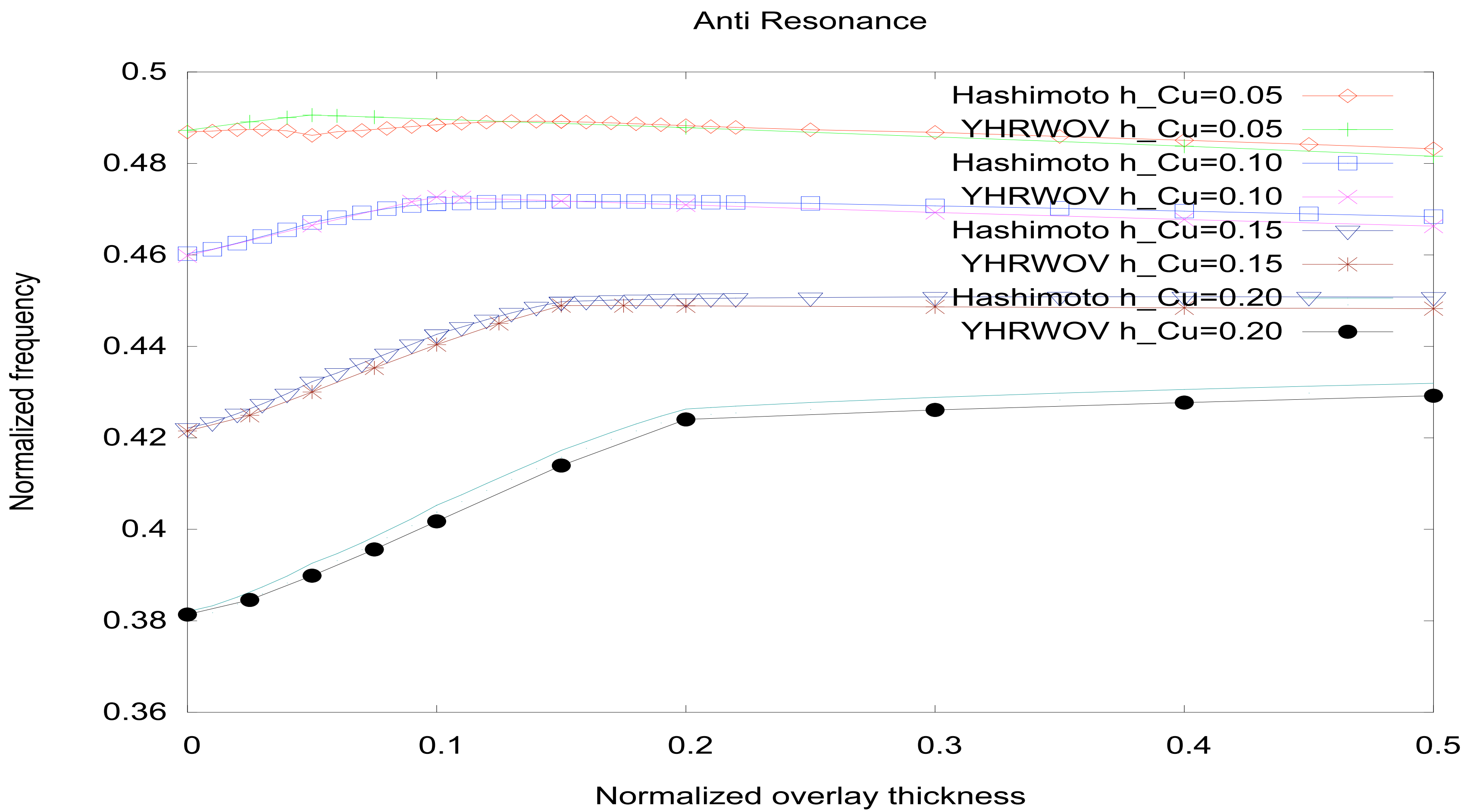

Conclusions

- A new numerical model has been developed to analyze the influence of a SiO_2 overlay deposited on a single periodic array of metallic electrodes
- It is incorporating :
  - the periodic harmonic Green's function concept
  - the Finite Element Method for the modelization of the mechanical behavior of both the metallic electrode and the SiO_2 overlay
  - An homogeneous relative dielectric permittivity has been assumed for the upper half space and computed using FreeFEM ++ package
  - Comparison with K. Hashimoto's study of the influence of the SiO2 overlay thickness on the Resonant and Anti-Resonant frequencies of a single periodic array is satisfactory

Future Work

- Full simutation of the electro-acoustical problem using FreeFem++
- Extend to 3D model : incorporate transversal effects