Note jotted down using Xournal++:

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Notes on Thesis Topics

① Extended Conductivity model:

Issue: Eddy current model with conductivity $\sigma = \sigma(x)$ smoothly varying and locally vanishing (SVLV)

Frequency domain: [eddy current model]

$$\operatorname{curl} E = i\omega\mu H$$
$$\operatorname{curl} H = \sigma(x) E + j_s$$

↑ conductivity

$$\mu H = \operatorname{curl} A$$
$$E = -i\omega A - \operatorname{grad}\phi$$

$$\triangleright \quad \operatorname{curl}\mu^{-1}\operatorname{curl} A + i\omega\sigma(x) A + i\omega\sigma(x)\operatorname{grad}\phi = j_s$$
$$\operatorname{div} A = 0$$

Problem already affects stationary conduction model:

For crisply defined conductor, occupying Ω_C:

$\Omega_C \hat{=}$ conducting region, $\sigma \geq \sigma_0 > 0$

$\Omega_I \hat{=}$ insulating region $\sigma = 0$

$\phi \hat{=}$ electric potential

(I) In Ω_C: $-\operatorname{div}\sigma(x)\operatorname{grad}\phi_{|\Omega_C} = 0$

(II) In Ω_I: $-\operatorname{div}\epsilon(x)\operatorname{grad}\phi_{|\Omega_I} = 0$

\+ voltage excitation by boundary conditions

\+ Zero-flux conditions on $\partial\Omega_C$

If σ can become arbitrarily small then even defining Ω_C becomes problematic.

$\triangleright$ Model breaks down for σ SVLV

Mobile charge carrier model (drift-diffusion)

$n = n(x) \triangleq$ density of mobile electrons $[n] = m^{-3}$

$c = c(x) \triangleq$ density of immobile positive charges $[c] = m^{-3}$

known can also be SVLV

Drift-diffusion current law:

$$j_n(x) = q\, n\,(\underbrace{D \operatorname{grad} n(x)}_{\text{electron diffusion}} - \underbrace{\mathcal{M} E(x)}_{\text{drift}})\,, \quad [j_n] = \frac{A}{m^2}$$

q: particle charge $[q] = As$

E: electric field

$\mathcal{M} \triangleq$ mobility (friction coefficient), $[\mathcal{M}] = \frac{V}{s} m^2$

$D \triangleq$ diffusivity,

Neutrality constraint:

$$\int_\Omega n(x)\,dx = \int_\Omega c(x)\,dx$$

Full model [ε constant, $\equiv 1$]

$$\boxed{\left\{\begin{array}{rl} -\Delta \phi &= c - n \\ j &= n\,(D \operatorname{grad} n - \mathcal{M} \operatorname{grad} \phi) \quad \text{in } \Omega \\ \operatorname{div} j &= 0 \quad \text{[charge conservation]} \end{array}\right.}$$

+ "artificial" boundary conditions for ϕ:

$$\phi = \phi_D \quad \text{on } \Gamma_D \subset \partial\Omega$$

$$\operatorname{grad}\phi \cdot n = 0 \quad \text{on } \Gamma_N \subset \partial\Omega$$

to be implemented

+ electron injection at contacts: $n = n_D$ on Γ_D

+ no-flux condition at insulating contacts: $j \cdot n = 0$ on Γ_N

The **drift–diffusion model** of electrical transport plays a major role in describing the current flow in semiconductors. It takes into account contributions from electrons and holes. This page concentrates on the former.

Under an external voltage applied to the semiconductor material, electrons in the conduction bands tend to move toward the positive electrode. The average velocity of electrons $\mathbf{v}_d$ is known as the **drift velocity**, and it contributes to the current as $J_n = qn\mathbf{v}_d = qn\mu_n E$, where μ_n is the mobility of electrons, and E is the electric field.

Diffusion is another mechanism that contributes to the flow of the current, even in the absence of external fields. It exists when the carrier concentration is not constant throughout the semiconductor, i.e., when there is a gradient of carrier concentration. Diffusion contributes to the current as $J_n = qD_n \nabla n$, where D_n is the diffusion coefficient. A full description of the transport in semiconductors also requires continuity equations for electrons and holes:

$$\frac{\partial n}{\partial t} - \frac{1}{q}\nabla \cdot J_n = \frac{\partial p}{\partial t} + \frac{1}{q}\nabla \cdot J_p = -R(\psi, n, p)$$

where ψ is the electrostatic potential, defined as $E = -\nabla\psi$, and R is the net generation–recombination rate of electron–hole pairs per unit volume. The contributions to the electron and hole currents from drift and diffusion are

$$J_n = qn\mu_n E + qD_n \nabla_n, \quad J_p = qp\mu_p E - qD_p \nabla_p$$

The above system of equations is supplemented by the Poisson equation $-\nabla \cdot (\varepsilon \nabla \psi) = q(p - n - C)$, where C is the net impurity concentration, which is essentially independent of time. The diffusion coefficients and mobilities are related by the Einstein relations for electrons and holes:

$$\frac{D_n}{\mu_n} = \frac{k_B T}{q}, \quad \frac{D_p}{\mu_p} = \frac{k_B T}{q}$$

Limit model :

- Constant material properties
- $c \longrightarrow \infty$

Determine $D = D(c)$, $M = M(c)$, $n_D = n_D(c)$ such that

$\phi \longrightarrow \phi_\infty$, where ϕ_∞ solves

limit model

$$\begin{cases} -\operatorname{div} \sigma \operatorname{grad} \phi_\infty = 0 & \text{in } \Omega \\ \phi_\infty = \phi_D & \text{on } \Gamma_D \\ \operatorname{grad} \phi_\infty \cdot n = 0 & \text{on } \Gamma_N \end{cases}$$

Related work :

- P. Degond et. al about asymptotics-preserving schemes and quasi-neutral limits.

MR2390995 Reviewed Degond, Pierre; Liu, Jian-Guo; Vignal, Marie-Hélène Analysis of an asymptotic preserving scheme for the Euler-Poisson system in the quasineutral limit. *SIAM J. Numer. Anal.* 46 (2008), no. 3, 1298–1322. (Reviewer: Christian Dogbe) 82D10 (76N20 76W05 76X05)

MR2342122 Reviewed Choquet, Isabelle; Degond, Pierre; Lucquin-Desreux, Brigitte A hierarchy of diffusion models for partially ionized plasmas. *Discrete Contin. Dyn. Syst. Ser. B* 8 (2007), no. 4, 735–772. (Reviewer: Stephen Wollman) 76X05 (35Q35 76P05 82C70 82D10)

MR2314389 Reviewed Crispel, Pierre; Degond, Pierre; Vignal, Marie-Hélène An asymptotic preserving scheme for the two-fluid Euler-Poisson model in the quasineutral limit. *J. Comput. Phys.* 223 (2007), no. 1, 208–234. 76X05 (65M99 82D10)

MR2139410 Reviewed Degond, Pierre; Jin, Shi A smooth transition model between kinetic and diffusion equations. *SIAM J. Numer. Anal.* 42 (2005), no. 6, 2671–2687. (Reviewer: Alexander Orlov) 82B40 (65M55 76R50 82C40 82C80)

MR1880746 Reviewed Degond, P.; Klar, A. A relaxation approximation for transport equations in the diffusive limit. *Appl. Math. Lett.* 15 (2002), no. 2, 131–135. 35F20 (35B25 82C70)

▷ Probably more works on this ?

② Hodge-Helmholtz equation in the stationary limit. (Singular perturbation)

2D: Hodge-Helmholtz BVP, $\omega > 0$

- PDE: $\underline{\mathrm{curl}}_{2D}\, \mathrm{curl}_{2D}\, \underline{u} - \mathrm{grad}\, \mathrm{div}\, \underline{u} - \omega^2 \underline{u} = \underline{f}$

3D: $\mathrm{curl}\, \mathrm{curl}\, \underline{u} - \mathrm{grad}\, \mathrm{div}\, \underline{u} - \omega^2 \underline{u} = \underline{f}$

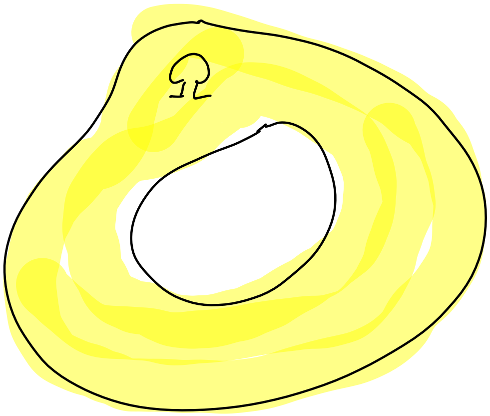
- Dirichlet boundary conditions:

  $\underline{u}_t$ and $\mathrm{div}\, \underline{u}$ prescribed on boundary

  tangential component

- Neumann boundary conditions:

  $\underline{u}_n$ and $\mathrm{curl}\, \underline{u}$ prescribed on boundary



If Ω has a hole, $\beta_1(\Omega) > 0$, then for $\omega = 0$ the BVPs will fail to possess a unique solution: finite-dimensional nullspaces spanned by Dirichlet-/Neumann harmonic vectorfields.

However: For general domains harmonic vectorfields are complicated and not easily computed.

Challenge: BVPs have unique solutions for $\omega \neq 0$ sufficiently small, but not for $\omega = 0$

How to stabilize discrete models for $\omega \to 0$?
How to solve FE models efficiently for $\omega \approx 0$?

Based on curl-conforming FE & mixed variational formulation.

Related : Neumann problem

$$\begin{cases} -\Delta u + \omega^2 u = f & \text{in } \Omega \\ \operatorname{grad} u \cdot n = 0 \end{cases}$$

$\omega = 0$ $\triangleright$ uniqueness of solutions lost

Nullspace = constants
[simple & known]

$\triangleright$ stabilized variational formulation

$$\int_\Omega \operatorname{grad} u \cdot \operatorname{grad} v + \omega^2 u v \, dx = \int_\Omega f v \, dx \quad \forall v \in H^1(\Omega)$$

$$\int_\Omega u \, dx = 0 .$$

③ PUM-Based Wave-Ray Multigrid

↳ PUM ≙ partition of unity

We consider the following Helmholtz boundary value problem posed on a two-dimensional domain $\Omega \subset \mathbb{R}^2$:

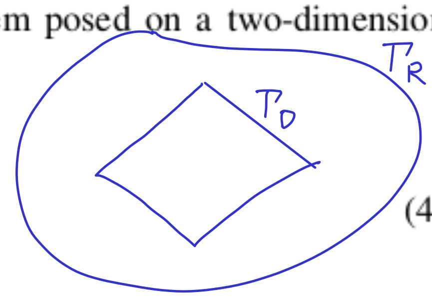


Fig. 4.1.

$$\begin{aligned} \Delta u + k^2 &= 0 \quad \text{in } \Omega \,, \\ \frac{\partial u}{\partial \boldsymbol{n}} - iku &= g \quad \text{on } \Gamma_R \,, \\ u &= 0 \quad \text{on } \Gamma_D \,. \end{aligned} \tag{4.1}$$

Here, $k > 0$ is the wavenumber, and Γ_D and Γ_R are two well separated parts of the boundary, $\Gamma_R \cup \Gamma_D = \partial\Omega$, see Figure 4.1. The boundary value problem (4.1) has a variational formulation in $H^1_{\Gamma_D}(\Omega)$: $\mathsf{a}(u, v) = \ell(v)$ for all $v \in H^1_{\Gamma_D}(\Omega)$.

Discretization on a fine triangular mesh $\mathcal{T}_L$ is based on piecewise linear Lagrangian finite elements (space $\mathcal{S}^0_1(\mathcal{T}_L)$) with zero boundary conditions on Γ_D). Further we assume a hierarchy of nested meshes $\mathcal{T}_0 \prec \mathcal{T}_1 \prec \cdots \prec \mathcal{T}_L$ created by uniform, regular refinement.

Let $\mathcal{V}_l$ denote the set of vertices of $\mathcal{T}_l$ not lying on Γ_D. Write $b^l_{\boldsymbol{p}}$ for the piecewise linear nodal basis function ("tent function") associated with vertex $\boldsymbol{p} \in \mathcal{V}_l$. Write

$$\boldsymbol{d}^m_k = \begin{pmatrix} \cos \frac{2\pi}{m} k \\ \sin \frac{2\pi}{m} k \end{pmatrix} , \quad k = 0, \ldots, m-1 \,, \tag{4.2}$$

and define the wave modulated partition of unity space according to

$$\begin{aligned} W_L &:= \mathcal{S}^0_1(\mathcal{T}_L) \,, \\ W_l &:= \operatorname{span}\left\{ b^l_{\boldsymbol{p}}(\boldsymbol{x}) \underbrace{\exp(ik\boldsymbol{d}^{2^{L+1-l}}_k \cdot \boldsymbol{x})}_{\hookrightarrow \text{ plane wave !}} : \boldsymbol{p} \in \mathcal{V}_l,\ k = 0, \ldots, 2^{L+1-l} - 1 \right\} \,, \\ & l = 0, \ldots, L-1 \,. \end{aligned} \tag{4.3}$$

The following two level algorithm (correction scheme) is proposed for solving the variational problem on W_l, $l \geq 1$:

1. Conduct a directional Gauss-Seidel relaxation.
2. Solve the residual equation on W_{l-1} to obtain a correction.
3. Perform another directional Gauss-Seidel relaxation.

The directional Gauss-Seidel relaxation is based on the following ordering of the degrees of freedom:

- D.o.f. are first ordered according to the direction $\boldsymbol{d}$ they are associated with
- D.o.d. belonging to the same direction are partially ordered in *upstream fashion* with respect to that direction.

▷ Since the spaces W_ℓ are not nested suitable transfer operators for residuals and corrections are not straightforward.

Idea: "Adjacent directions"

Implementation in LehrFEM++

References:

[1] A. Brandt and I. Livshits, *Wave ray multigrid method for standing wave equations*, ETNA, 6 (1997), pp. 162–181.

[2] B. Lee, T. Manteuffel, S. McCormick, and J. Ruge, *Multilevel first order system least squares (FOSLS) for Helmholtz equations*, SIAM J. Sci. Comp., (1999). To appear.

[3] I. Livshits, *An algebraic multigrid wave-ray algorithm to solve eigenvalue problems for the Helmholtz operator*, Numer. Linear Algebra and Applications, 11 (2004), pp. 229–239.

[4] I. Livshits and A. Brandt, *Accuracy properties of the wave-ray multigrid algorithm for Helmholtz equations*, SIAM J. Sci. Comp., 28 (2006), pp. 1228–1251.

PUM:

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More recent work available

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Numer. Linear Algebra Appl. 26 (2019), no. 1, e2206, 19 pp.