

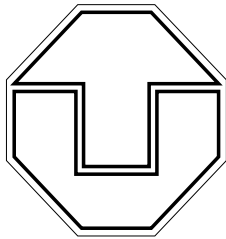
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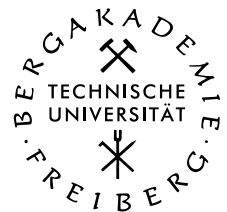
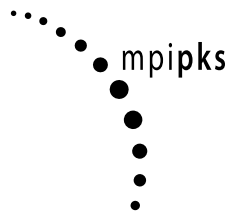
M. Hinze and R. Pinnau

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A Second Order Approach to Optimal Semiconductor Design

Michael Hinze

Institut für Numerische Mathematik,
Technische Universität Dresden
D-01069 Dresden, Germany,
email: hinze@math.tu-dresden.de

René Pinnau

Fachbereich Mathematik,
Technische Universität Kaiserslautern
D-67663 Kaiserslautern, Germany,
email: pinnau@mathematik.uni-kl.de

Abstract

Second order methods for optimal semiconductor design based on the standard drift diffusion model are developed. Second-order necessary and sufficient conditions are established. Local quadratic convergence for Newton's method is proved. Numerical results for an unsymmetric n-p-diode are presented.

Key words. Semiconductor design, drift diffusion, optimal control, second-order necessary and sufficient conditions, KKT systems, Newton's method, numerics.

AMS(MOS) subject classification. 35J50, 49J20, 49K20, 90C48.

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1 Introduction

The accelerating miniaturization in semiconductor industry had during the last decades a strong impact on the development of sophisticated semiconductor models and numerical methods, which are implemented in the common simulation tools. Clearly, this branch of research will be getting even stronger during the next years, as can be seen from the projection of the Semiconductor Industry Association (SIA), which says that by 2009 the leading edge MOS device will employ a $0.05\ \mu\text{m}$ length scale and an oxide thickness of 1.5 nm or less. This has the direct consequence, that the design cycle for next product generation will shorten from year to year, such that some optimized design for a semiconductor device cannot be found straightforwardly using just cumbersome and time consuming simulations.

During the last years a new branch of research developed aiming at the automated optimal design of semiconductor devices, where we can distinguish mainly two approaches. The engineering community was focussing on black box algorithms and nonlinear least squares approaches [Cia01, DKKS96, Kha95, KFBS95, PSSS98, LWT99, Sto00, SSP+98, SSP+99], which were attached to advanced simulation tools. Meanwhile, the applied mathematics community employed techniques from infinite dimensional constrained optimization, which are also exploiting the special structure of the underlying semiconductor models [BEMP01, BEM02, FC92, FI92, BFI93, FI94, HP01, HP02, BP03]. This lead to an significant improvement concerning the overall simulation times, since the performance of these methods is by construction independent of the number of design parameters.

Although there exists a whole hierarchy of macroscopic semiconductor models, most of these optimization approaches are based on the well-known drift diffusion (DD) model for semiconductor devices [Sze81, Sel84, MRS90, Jün01]. This is clearly related to the great success of this model and to the fact that there exists a vast literature on analytical and numerical results concerning the underlying model equations (cf. [CPB00] and the references therein).

The main objective in optimal semiconductor design is to get an improved current flow at a specific contact of the device, e.g. focusing on the reduction of the leakage current in MOSFET devices or maximizing the drive current [SSP+98]. In both cases a certain working point is fixed and one tries to achieve the objective by a change of the doping profile. An overview on the mathematical tools employed for the solution of this design question can be found in [HP05].

So far, most numerical optimization approaches were using steepest descent methods relying on first-order derivative information. Although performing already very successfully, they show as expected only first order convergence. Here, we will go one step further and devise a numerical algorithm based on Newton's method, which shows the desired second order convergence behavior. Using the adjoint variables we construct the algorithm in such a way that we only need applications of the Hessian avoiding storage restrictions. This approach ensures that the overall method is independent of the number of design parameters, in contrast to black box methods based on sensitivities.

The paper is organized as follows. In the remainder of this section we will introduce the DD model including generation–recombination rates. Then, in Section 2 we specify the optimal control problem, its analytical setting and give an existence result. The first–order and second–order optimality system is studied in Section 3, where we also analyze second order sufficiency conditions. The Newton algorithm is introduced in Section 4 and its local convergence is proved. Lastly, numerical results for an unsymmetric n–p–diode are presented in Section 5, which underline the feasibility of our approach.

1.1 The Drift Diffusion Model

The stationary standard DD model for semiconductor devices stated on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$, or 3 reads

$$J_n = q(D_n \nabla n + \mu_n n \nabla V), \quad (1.1a)$$

$$J_p = -q(D_p \nabla p - \mu_p p \nabla V), \quad (1.1b)$$

$$\operatorname{div} J_n = qR(n, p), \quad (1.1c)$$

$$\operatorname{div} J_p = -qR(n, p), \quad (1.1d)$$

$$-\epsilon \Delta V = q(n - p - C). \quad (1.1e)$$

The unknowns are the densities of electrons $n(x)$ and holes $p(x)$, the current densities of electrons $J_n(x)$ and holes $J_p(x)$, respectively, and the electrostatic potential $V(x)$. The total current density is given by

$$J = J_n + J_p. \quad (1.1f)$$

The doping profile is denoted by $C(x)$. The parameters D_n, D_p, μ_n, μ_p are the diffusion coefficients and mobilities of electrons and holes respectively. The physical constants are the elementary charge q and the materials permittivity constant ϵ .

The function $R(n, p)$ models the rate of generation and recombination of electron–hole carrier pairs. There exist various energy transition processes which can lead to recombination–generation, which can be modeled e.g. by the *Shockley–Read–Hall* term

$$R_{SRH}(n, p) = \frac{np - n_i^2}{\tau_p^l(n + n_i) + \tau_n^l(p + n_i)},$$

where τ_n^l and τ_p^l are the electron and hole lifetimes, respectively. Another recombination–generation process is described by the *Auger* term

$$R_{AU}(n, p) = (a_1 n + a_2 p)(np - n_i^2).$$

Remark 1.1. There are also sole generation processes like *impact ionization* [Sze81] which we will not consider here.

In the following we only consider regimes in which we can assume the Einstein relations

$$D_n = U_T \mu_n, \quad D_p = U_T \mu_p,$$

where $U_T = k_B T/q$ is the thermal voltage of the device and T denotes its temperature and k_B the Boltzmann constant. Further, let the mobilities be constant excluding a dependence on the electric field.

System (1.1) is supplemented with the following boundary conditions: We assume that the boundary $\partial\Omega$ of the domain Ω splits into two disjoint parts Γ_D and Γ_N , where Γ_D models the Ohmic contacts of the device and Γ_N represents the insulating parts of the boundary. Let ν denote the unit outward normal vector along the boundary. First, assuming charge neutrality and thermal equilibrium at the Ohmic contacts Γ_D and, secondly, zero current flow and vanishing electric field at the insulating part Γ_N yields the following set of boundary data

$$n = n_D, \quad p = p_D, \quad V = V_D \quad \text{on } \Gamma_D, \quad (1.1g)$$

$$J_n \cdot \nu = J_p \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N, \quad (1.1h)$$

where n_D, p_D, V_D are the $H^1(\Omega)$ -extensions of

$$n_D = \frac{C + \sqrt{C^2 + 4n_i^2}}{2}, \quad p_D = \frac{-C + \sqrt{C^2 + 4n_i^2}}{2},$$

$$V_D = -U_T \log\left(\frac{n_D}{n_i}\right) + U, \quad \text{on } \Gamma_D.$$

Here, U denotes the applied biasing voltage and n_i the intrinsic carrier density of the semiconductor.

To rewrite the equations in nondimensional form we employ the following diffusion scaling

$$\begin{aligned} n &\rightarrow C_m \tilde{n}, & p &\rightarrow C_m \tilde{p}, & x &\rightarrow L \tilde{x}, \\ C &\rightarrow C_m \tilde{C}, & V &\rightarrow U_T \tilde{V}, & J_{n,p} &\rightarrow \frac{q U_T C_m \mu_{n,p}}{L} \tilde{J}_{n,p} \end{aligned}$$

where L denotes a characteristic device length, C_m the maximal absolute value of the background doping profile and $\mu_{n,p}$ a characteristic value for the respective mobilities. Defining the dimensionless *Debye length*

$$\lambda^2 = \frac{\epsilon U_T}{q C_m L^2}$$

the scaled equations read

$$\operatorname{div} J_n = R(n, p), \quad J_n = \nabla n + n \nabla V, \quad (1.2a)$$

$$\operatorname{div} J_p = -R(n, p), \quad J_p = -(\nabla p - p \nabla V), \quad (1.2b)$$

$$-\lambda^2 \Delta V = n - p - C, \quad (1.2c)$$

where we omitted the tilde for notational convenience. The Dirichlet boundary conditions transform to

$$n_D = \frac{C + \sqrt{C^2 + 4\delta^4}}{2}, \quad p_D = \frac{-C + \sqrt{C^2 + 4\delta^4}}{2}, \quad (1.2d)$$

$$V_D = -\log\left(\frac{n_D}{\delta^2}\right) + U, \quad \text{on } \Gamma_D, \quad (1.2e)$$

where $\delta^2 = n_i/C_m$ denotes the scaled intrinsic density.

Remark 1.2. Clearly, also the scaled parameter function R has to be expressed in terms of the scaled variables. The scaled Shockley–Read–Hall recombination–generation term then reads for example

$$R_{SRH}(n, p) = \frac{np - \delta^4}{\tau_p^l(n + \delta^2) + \tau_n^l(p + \delta^2)}.$$

For the subsequent considerations we pose the following assumptions.

- A.1** Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or 3 be a bounded domain with boundary $\partial\Omega \in C^{0,1}$. The boundary $\partial\Omega$ is piecewise regular and splits into two disjoint parts Γ_N and Γ_D . The set Γ_D has nonvanishing $(d - 1)$ -dimensional Lebesgue–measure. Γ_N is closed.
- A.2** Let $\Gamma_D = \bigcup_{l=1}^M \Gamma_D^l$, $M \geq 2$ and $\text{dist}(\Gamma_D^{l_1}, \Gamma_D^{l_2}) > 0$ for $l_1 \neq l_2$ and $l_1, l_2 \in \{1, \dots, M\}$. It holds $\Gamma_O = \bigcup_{k=1}^N \Gamma_D^{l_k}$ for $1 \leq N \leq M$.
- A.3** The boundary data fulfill $(n_D, p_D, V_D) \in H^1(\Omega)$.
- A.4** The recombination–generation term is of the form $R(n, p) = R_1(n, p)(np - \delta^4)$, where $R_1 : \mathbb{R}^2 \rightarrow \mathbb{R}_0^+$ is twice continuously differentiable with locally Lipschitz continuous second derivatives.

Remark 1.3. Assumptions **A.1**–**A.3** are necessary for the regularity of solutions of the state system. Note, that **A.2** is also physically reasonable, since it prevents short–circuiting. Further, the Shockley–Read–Hall and the Auger recombination–generation terms clearly fulfill **A.4**.

1.2 Properties of the State System

In [HP02] system (1.2) was treated after eliminating the current densities J_n and J_p , which was most convenient for a first–order approach and which is also the standard treatment for the analysis of this system [Mar86]. Considering the numerical treatment of system (1.2), we want to point out that the standard Scharfetter–Gummel discretization [SG69] can be interpreted as a mixed finite element discretization of the state system [GMS98]. For the second–order approach we are going to introduce here, we also use this mixed

formulation, since this has several advantages for the analytical study. For this reason we redefine a new state space as follows

$$X \stackrel{\text{def}}{=} [L^2(\Omega)]^d \times [L^2(\Omega)]^d \times (x_D + X_0),$$

where $x_D \stackrel{\text{def}}{=} (n_D, p_D, V_D)$ denotes the boundary data introduced in (1.2) and $X_0 \stackrel{\text{def}}{=} [H_{0,\Gamma_D}^1(\Omega) \cap L^\infty(\Omega)]^3$. Then, the space X is equipped with the norm

$$\|x\|_X \stackrel{\text{def}}{=} \|(x_1, x_2)\|_{[L^2(\Omega)]^{2d}} + \|(x_3, x_4, x_5)\|_{[H^1(\Omega)]^3} + \|(x_3, x_4, x_5)\|_{[L^\infty(\Omega)]^3}$$

yielding a Banach space, where we define the space of Sobolev functions with vanishing trace along Γ_D via

$$H_{0,\Gamma_D}^1(\Omega) \stackrel{\text{def}}{=} \{\phi \in H^1(\Omega) : \phi|_{\Gamma_D} = 0\}.$$

The set of co-states will then be $Z \stackrel{\text{def}}{=} [L^2(\Omega)]^d \times [L^2(\Omega)]^d \times [H^1(\Omega)]^3$ and the set of admissible controls is given by

$$\mathcal{C} \stackrel{\text{def}}{=} \{C \in H^1(\Omega) : C = \bar{C} \text{ on } \Gamma_D\}. \quad (1.3)$$

We abbreviate the state variables as $x \stackrel{\text{def}}{=} (J_n, J_p, n, p, V)$ and rewrite the state equations (1.2) in the operator form $e(x, C) = 0$, where the nonlinear mapping $e : X \times \mathcal{C} \rightarrow Z^*$ is defined by

$$e(x, C) \stackrel{\text{def}}{=} \begin{pmatrix} J_n - (\nabla n + n \nabla V) \\ J_p + (\nabla p - p \nabla V) \\ \operatorname{div} J_n - R(n, p) \\ \operatorname{div} J_p + R(n, p) \\ -\lambda^2 \Delta V - n + p + C \end{pmatrix}. \quad (1.4)$$

There are various results on the solvability of the state system for different assumptions on the mobilities and on the recombination-generation terms (c.f. [Moc83, Mar86, MRS90] and the references therein). For completeness we state the the following existence results, for which the proof can be found in [NW91].

Proposition 1.4. *Assume A.1–A.4. Then for each $C \in H^1(\Omega)$ and all boundary data (n_D, p_D, V_D) with*

$$\frac{1}{K} \leq n_D(x), p_D(x) \leq K, \quad x \in \Omega, \quad \text{and} \quad \|V_D\|_{L^\infty(\Omega)} \leq K$$

for some $K \geq 1$, there exists a solution $(J_n, J_p, n, p, V) \in [L^2(\Omega)]^2 \times (H^1(\Omega) \cap L^\infty(\Omega))^3$ of system (1.2) fulfilling

$$\frac{1}{L} \leq n(x), p(x) \leq L, \quad x \in \Omega, \quad \text{and} \quad \|V\|_{L^\infty(\Omega)} \leq L$$

for some constant $L = L(\Omega, K, \|C\|_{L^p(\Omega)}) \geq 1$, where the embedding $H^1(\Omega) \hookrightarrow L^p(\Omega)$ holds.

Remark 1.5. Compared to the existence result given in [Mar86] we need this refined version, since the doping profile is acting as the control parameter in our setting and the coercivity of the cost functional will later on allow to derive precisely the bounds on C stated in the proposition.

Next, we state a result on the differentiability properties of the mapping e which extends the result given in [HP02, Theorem 3.3] to the mixed formulation including now also recombination–generation terms. We omit the proof since it is a straightforward extension of the previously mentioned result.

Theorem 1.6. *The mapping e defined in (1.4) is infinitely often Fréchet differentiable with derivatives vanishing for order greater than 2. The actions of the first derivatives at a point $(x, C) \in X \times \mathcal{C}$ in a direction $\hat{x} = (\hat{J}_n, \hat{J}_p, \hat{n}, \hat{p}, \hat{V}) \in [L^2(\Omega)]^d \times [L^2(\Omega)]^d \times X_0$ are given by*

$$\begin{aligned} \langle e_x(x, C)\hat{x}, z \rangle_{Z^*, Z} &= \left\langle \hat{J}_n - \left(\nabla \hat{n} + \hat{n} \nabla V + n \nabla \hat{V} \right), z^n \right\rangle_{L^2, L^2} \\ &+ \left\langle \hat{J}_p + \left(\nabla \hat{p} - \hat{p} \nabla V - p \nabla \hat{V} \right), z^p \right\rangle_{L^2, L^2} + \left\langle \operatorname{div} \hat{J}_n - R_n \hat{n} - R_p \hat{p}, z^{J_n} \right\rangle_{(H^1)^*, H^1} \\ &+ \left\langle \operatorname{div} \hat{J}_p + R_n \hat{n} + R_p \hat{p}, z^{J_p} \right\rangle_{(H^1)^*, H^1} + \left\langle -\lambda^2 \Delta \hat{V} - \hat{n} + \hat{p}, z^V \right\rangle_{(H^1)^*, H^1} \end{aligned} \quad (1.5)$$

for all $z = (z^n, z^p, z^{J_n}, z^{J_p}, z^V) \in Z$.

Further, we have

$$\left\langle e_C(x, C)\hat{C}, z \right\rangle_{(H^1)^*, H^1} = \left\langle \hat{C}, z^V \right\rangle_{(H^1)^*, H^1} \quad (1.6)$$

for all $\hat{C} \in H_{0, \Gamma_D}^1(\Omega)$ and $z \in Z$.

The second derivatives $e_{xC}(x, C)$, $e_{Cx}(x, C)$ and $e_{CC}(x, C)$ vanish, the action of the second derivative w.r.t. x at point (x, C) in directions $\hat{x}_1 = (\hat{J}_{n1}, \hat{J}_{p1}, \hat{n}_1, \hat{p}_1, \hat{V}_1)$, $\hat{x}_2 = (\hat{J}_{n2}, \hat{J}_{p2}, \hat{n}_2, \hat{p}_2, \hat{V}_2) \in X_0$ is given by

$$\begin{aligned} \langle e_{xx}(x, C)(\hat{x}_1, \hat{x}_2), z \rangle_{Z^*, Z} &= \left\langle \hat{n}_1 \nabla \hat{V}_2 + \hat{n}_2 \nabla \hat{V}_1, z^n \right\rangle_{L^2, L^2} - \left\langle \hat{p}_1 \nabla \hat{V}_2 + \hat{p}_2 \nabla \hat{V}_1, z^p \right\rangle_{L^2, L^2} \\ &+ \left\langle R_{nn} \hat{n}_1 \hat{n}_2 + R_{np} \hat{n}_1 \hat{p}_2 + R_{np} \hat{n}_2 \hat{p}_1 + R_{pp} \hat{p}_1 \hat{p}_2, z^{J_p} - z^{J_n} \right\rangle_{(H^1)^*, H^1} \end{aligned} \quad (1.7)$$

for all $z = (z^n, z^p, z^{J_n}, z^{J_p}, z^V) \in Z$.

Here, we denote the duality pairing of a Banach space W with its dual W^* by $\langle \cdot, \cdot \rangle_{W^*, W}$.

2 The Optimization Problem

In this section we want to give the precise mathematical statement of the optimization problem under investigation.

We are going to minimize cost functionals of the form

$$Q(J_n, J_p, n, p, V, C) \stackrel{\text{def}}{=} Q_1(J_n, J_p) + \frac{\gamma}{2} \int_{\Omega} |\nabla(C - \bar{C})|^2 dx, \quad (2.1)$$

where \bar{C} is a given reference doping profile and the parameter γ allows to adjust the deviations from \bar{C} . One is mainly interested in functionals Q_1 , which depend only on the values of the outflow current density on some contact Γ_O

$$Q_1(J_n, J_p) = S(J \cdot \nu|_{\Gamma_O}). \quad (2.2)$$

Remark 2.1. In [HP02], the functional under investigation was

$$S(J \cdot \nu|_{\Gamma_O}) = \frac{1}{2} \|(J - J^*) \cdot \nu\|_{(H_{00}^{1/2}(\Gamma_O))^*}^2, \quad (2.3)$$

corresponding to the objective of finding an outflow current density $J \cdot \nu$ close to a desired density $J^* \cdot \nu$. In [BP03] the total current flow on a contact is studied, i.e.

$$S(J \cdot \nu|_{\Gamma_O}) = \frac{1}{2} \left| \int_{\Gamma_O} J \cdot \nu ds - I^* \right|^2 \quad (2.4)$$

(for some desired current flow I^*). Note that especially in the one dimensional setting these two functionals are equivalent.

The objective of the optimization, the current flow over a contact Γ_O , is given by

$$I = \int_{\Gamma_O} J \cdot \nu ds = \int_{\Gamma_O} (J_n + J_p) \cdot \nu ds. \quad (2.5)$$

In [HP05] it was pointed out that there might be multiple solutions if this objective is considered, since in the optimum one might change the roles of electrons and holes, which both contribute to the total current density J . Clearly, this can lead to significant convergence problems in the numerical algorithms. For this reason we split the desired current flow into two parts

$$I_n = \int_{\Gamma_O} J_n \cdot \nu ds, \quad I_p = \int_{\Gamma_O} J_p \cdot \nu ds \quad (2.6)$$

and consider especially in the numerical investigations the following objective

$$S(J_n \cdot \nu|_{\Gamma_O}, J_p \cdot \nu|_{\Gamma_O}) = \frac{1}{2} \left| \int_{\Gamma_O} J_n \cdot \nu ds - I_n^* \right|^2 + \frac{1}{2} \left| \int_{\Gamma_O} J_p \cdot \nu ds - I_p^* \right|^2 \quad (2.7)$$

Although this is sound from the mathematical point of view one has to emphasize that it is physically impossible to measure the electron and hole current separately.

The optimization problem we investigate in the present research is then given by

$$\min_{X \times C} Q(x, C) \quad \text{s.t.} \quad e(x, C) = 0. \quad (2.8)$$

For the following analytical and numerical investigations we also need some regularity assumptions on the cost functional:

A.5 Let $Q : X \times \mathcal{C} \rightarrow \mathbb{R}$ denote a cost functional which is twice continuously Fréchet differentiable with Lipschitz continuous second derivatives. Further, let Q be of separated type, i.e. $Q(x, C) = Q_1(x) + Q_2(C)$ and radially unbounded w.r.t. \mathcal{C} for every $x \in X$, bounded from below and weakly lower semi-continuous.

Remark 2.2. Assumption **A.5** is standard for the construction of second-order optimization methods [HK01]. We note that it is especially fulfilled for the objective function (2.7).

The existence of a minimizer is proved in [HP02] under mild assumptions on the cost functional Q and when the state system is given with respect to the unknowns (n, p, V) without recombination-generation terms. This proof can be easily extended to the mixed formulation including recombination-generation terms given by (1.2) yielding the following existence result.

Theorem 2.3. *The constrained minimization problem (2.8) admits at least one solution $(J_n^*, J_p^*, n^*, p^*, V^*, C^*) \in X \times \mathcal{C}$.*

Remark 2.4. In general, we cannot expect the uniqueness of a minimizer, since the optimization problem is non-convex due to the nonlinear constraint. Further, there exist analytical and numerical evidences that the optimization admits multiple solutions at least for special choices of the cost functional and of the reference doping profile \bar{C} . For details we refer to [HP05].

3 The First-order Optimality System and Second-order conditions

In this section we want to study the first-order optimality system and the second-order conditions for the optimization problem (2.8). We introduce the Lagrangian $\mathcal{L} : X \times \mathcal{C} \times Z \rightarrow \mathbb{R}$ associated to the minimization problem (2.8) which is defined by

$$\mathcal{L}(x, C, \xi) \stackrel{\text{def}}{=} Q(x, C) + \langle e(x, C), \xi \rangle_{Z^*, Z}.$$

It is an easy consequence of Theorem 1.6 and **A.5** that the Lagrangian \mathcal{L} is twice continuously Fréchet differentiable with Lipschitz continuous second derivatives.

3.1 The First Order Optimality System

The first order optimality condition corresponding to problem (2.8) is given by

$$\mathcal{L}'(x^*, C^*, \xi^*) = 0. \tag{3.1}$$

Rewriting (3.1) componentwise we get

$$e(x^*, C^*) = 0 \quad \text{in } Z^*, \quad (3.2a)$$

$$e_x^*(x^*, C^*)\xi^* + Q_x(x^*, C^*) = 0 \quad \text{in } X^*, \quad (3.2b)$$

$$e_C^*(x^*, C^*)\xi^* + Q_C(x^*, C^*) = 0 \quad \text{in } \mathcal{C}^*. \quad (3.2c)$$

Here, $e_C^*(x, C) \in L(Z, \mathcal{C}^*)$ and $e_x^*(x, C) \in L(Z, X^*)$ are continuous linear mappings denoting the adjoint operators associated to the linearized operators $e_C(x, C)$ and $e_x(x, C)$, respectively.

To write these equations in a more concise form we assume from now on that the cost functional Q is given via (2.7). Then, a direct calculation employing several integrations by parts leads to the following linear system for the adjoint variables $\xi = (\xi^n, \xi^p, \xi^{J_n}, \xi^{J_p}, \xi^V) \in Z$

$$\xi^n = \nabla \xi^{J_n}, \quad (3.3a)$$

$$\xi^p = \nabla \xi^{J_p}, \quad (3.3b)$$

$$\operatorname{div} \xi^n - \xi^n \nabla V = \xi^V + R_n \xi^{J_n} - R_n \xi^{J_p}, \quad (3.3c)$$

$$\operatorname{div} \xi^p + \xi^p \nabla V = \xi^V - R_p \xi^{J_n} + R_p \xi^{J_p}, \quad (3.3d)$$

$$-\lambda^2 \Delta V + \operatorname{div}(n \xi^n) + \operatorname{div}(p \xi^p) = 0, \quad (3.3e)$$

supplemented with the following set of boundary conditions

$$\xi^{J_n} = \begin{cases} \int_{\Gamma_O} J_n \cdot \nu \, ds - I_n^*, & \text{on } \Gamma_O, \\ 0, & \text{on } \Gamma_D \setminus \Gamma_O, \end{cases} \quad (3.4)$$

$$\xi^{J_p} = \begin{cases} - \left(\int_{\Gamma_O} J_p \cdot \nu \, ds - I_p^* \right), & \text{on } \Gamma_O, \\ 0, & \text{on } \Gamma_D \setminus \Gamma_O, \end{cases} \quad (3.5)$$

$$\xi^V = 0, \quad \text{on } \Gamma_D, \quad (3.6)$$

as well as

$$\xi^n \cdot \nu = \xi^p \cdot \nu = \nabla \xi^V \cdot \nu = 0 \quad \text{on } \Gamma_N. \quad (3.7)$$

Remark 3.1. Note, that it is possible to eliminate the Lagrange multipliers ξ^n and ξ^p employing the first two equations, which yields the system

$$\begin{aligned} \Delta \xi^{J_n} - \nabla \xi^{J_n} \nabla V &= \xi^V + R_n \xi^{J_n} - R_n \xi^{J_p}, \\ \Delta \xi^{J_p} + \nabla \xi^{J_p} \nabla V &= \xi^V - R_p \xi^{J_n} + R_p \xi^{J_p}, \\ -\lambda^2 \Delta V + \operatorname{div}(n \nabla \xi^{J_n}) + \operatorname{div}(p \nabla \xi^{J_p}) &= 0. \end{aligned}$$

For the existence of an Lagrange multiplier associated to an optimal solution $(x^*, C^*) \in X \times \mathcal{C}$ of (2.8) it is sufficient that the operator $e_{(x,C)}(x^*, C^*)$ is surjective. In general, this cannot be ensured for the drift diffusion model, since this system allows for multiple solutions, e.g. when one is considering thyristor devices [Moc83, Mar86]. Hence, we assume that the optimal solution is at least an isolated one, which excludes turning points in the current voltage characteristics.

A.6 For every minimizer $(x^*, C^*) \in X \times \mathcal{C}$ of Q the operator $e_x(x^*, C^*) : X \rightarrow Z^*$ admits a bounded inverse $e_x^{-1}(x^*, C^*) \in L(Z^*, X)$.

Remark 3.2. For the action of $e_x(x^*, C^*)$ see Theorem 1.6. One can prove that **A.6** holds near to the thermal equilibrium state, since there the solution is indeed unique. We note that for every minimizer (x^*, C^*) equation (3.2b) admits a unique solution $\xi^* \in Z$ due to assumption **A.6**. The function ξ^* is called Lagrange multiplier (associated to (x^*, C^*)).

3.2 The Second-order Condition

In order to formulate second-order conditions second derivatives of \mathcal{L} are required. It holds that

$$\mathcal{L}''(x, C, \xi) = \begin{bmatrix} Q_{xx}(x, C) + \langle e_{xx}(x, C)(\cdot, \cdot), \xi \rangle_{Z^*, Z} & 0 & e_x(x, C)^* \\ 0 & Q_{CC}(x, C) & e_c(x, C)^* \\ e_x(x, C) & e_c(x, C) & 0 \end{bmatrix}.$$

For notational convenience we define the state-control pair $y \stackrel{\text{def}}{=} (x, C)$ and $Y \stackrel{\text{def}}{=} X \times \mathcal{C}$. On the abstract level we get immediately the following result.

Theorem 3.3. *Let assumptions **A.1–A.6** be satisfied and let $y^* = (x^*, C^*)$ be an optimal solution to problem (2.8) with ξ^* denoting the associated Lagrange multiplier. Further, let $Q_{xx}(y^*)$ be positive semi-definite and $Q_{CC}(y^*)$ be positive definite. Then, $L_{yy}(y^*, \xi^*)$ is positive definite on $\ker e_y(y^*)$, provided $\|Q_x(y^*)\|_{X^*}$ is sufficiently small.*

Remark 3.4. Note, that the functional (2.1) with Q_1 given by (2.7) fulfills the assumptions of the theorem. Here, it is necessary to use the mixed formulation to get a functional which is quadratic in the current densities J_n and J_p , respectively. For the direct formulation with respect to (n, p, V) the functional S would be of fourth order with respect to the state variables and hence one would need to impose further assumptions on the observation to ensure the positive semi-definiteness of $Q_{xx}(y^*)$.

Proof: Let y^* be a minimizer of Q and denote the associated Lagrange multiplier by ξ^* . Since $e(y^*)$ is linear with respect to C we have $L_{CC}(y^*, \xi^*) = Q_{CC}(y^*)$. Now let $y = (x, C) \in \ker e_y(y^*)$. Then x and C satisfy

$$e_x(y^*)x = -e_c(y^*)C \text{ in } Z^*.$$

By Assumption **A.6** $e_x(y^*)$ admits a bounded inverse, such that the unique solution x of this equation satisfies

$$\|x\|_X \leq \kappa \|C\|_c$$

with some positive constant κ . Now since with $e_x^{-1}(y^*) \in L(Z^*, X)$ one has $e_x^{-*}(y^*) \in L(X^*, Z)$ such that using a similar argument as above we deduce from equation (3.2b)

$$\|\xi^*\|_Z \leq \tilde{\kappa} \|Q_x(y^*)\|_{X^*}.$$

Utilizing these estimates we obtain together with Assumptions **A.1–A.6**

$$\begin{aligned} \langle L_{yy}(y^*, \xi^*)y, y \rangle_{Y^*, Y} &= \langle L_{xx}(y^*, \xi^*)x, x \rangle_{X^*, X} + \langle Q_{CC}(y^*)C, C \rangle_{c^*, c} \\ &\geq \langle Q_{xx}(y^*)x, x \rangle_{X^*, X} + \langle e_{xx}(y^*)(x, x), \xi^* \rangle + \gamma \|C\|_c^2, \end{aligned}$$

since $Q_{CC}(y^*)$ is positive definite,

$$\geq -c \|x\|_X^2 \|\xi^*\|_Z + \gamma \|C\|_c^2,$$

due to (1.7),

$$\geq -c \|C\|_c^2 \|\xi^*\|_Z + \frac{\gamma}{2} \|C\|_c^2 + \frac{\gamma}{2} \|C\|_c^2,$$

since $e_x(y^*)$ is continuous,

$$\geq \left(-c \|Q_x(y^*)\|_{X^*} + \frac{\gamma}{2} \right) \|C\|_c^2 + \frac{\gamma}{2\sqrt{\kappa}} \|x\|_X^2$$

due to $x \in \ker e_x(y^*)$

$$\geq C \|y\|_Y^2,$$

if $\|Q_x(y^*)\|_{X^*}$ is sufficiently small. This concludes the proof.

4 Newton's Method for the Reduced Problem

It follows from assumption **A.6** together with the implicit function theorem that every solution (x^*, C^*) of problem (2.8) is locally unique. The same theorem then guarantees the unique solvability of the state equation $e(x, C) = 0$ in a neighborhood $\mathcal{U}(x^*, C^*) \stackrel{\text{def}}{=} \mathcal{U}_x(x^*) \times \mathcal{U}_C(C^*)$ and that $x = x(C) \in X$ for all $(x, C) \in \mathcal{U}(x^*, C^*)$ with x as function of C is as smooth as $e(x, C)$. In this case we can introduce the reduced cost functional $\hat{Q}(C) \stackrel{\text{def}}{=} Q(x(C), C)$ and problem (2.8) can locally be rewritten as

$$\min_{\mathcal{U}_C(C^*)} \hat{Q}(C), \tag{4.1}$$

where $x(C)$ is determined by $e(x(C), C) = 0$. Then, the derivative of the reduced cost functional is given by

$$\hat{Q}'(C) = Q_C(y(C)) + e_C^*(y(C))\xi, \quad (4.2)$$

where $\xi \in Z$ solves the adjoint equation $e_x^*(y(C))\xi = -Q_x(y(C))$ in Z^* .

We now derive Newton's method for problem (4.1). To begin with let $T : \mathcal{C} \rightarrow Y$,

$$T(y) \stackrel{\text{def}}{=} \begin{bmatrix} -e_x^{-1}(y)e_C(y) \\ Id_{\mathcal{C}} \end{bmatrix}.$$

Then, for $\xi \in Z$ the reduced Hessian is defined by

$$H(y, \xi) \stackrel{\text{def}}{=} T^*(y)L_{yy}(y, \xi)T(y), \quad H : \mathcal{C} \rightarrow \mathcal{C}, \quad (4.3)$$

and it holds that

$$H(y, C) = Q_{CC}(y) + e_C^*(y)e_x^{-*}(y) \{Q_{xx}(y)(\cdot, \cdot) + \langle e_{xx}(y)(\cdot, \cdot), \xi \rangle_{Z^*, Z}\} e_x^{-1}(y)e_C(y).$$

Proposition 4.1. *Let the assumptions of Theorem 3.3 be satisfied. Further, let $y^* = (x(C^*), C^*)$ denote a solution of problem (2.8), denote by ξ^* the associated Lagrange multiplier and let $\mathcal{U}(y^*) = \mathcal{U}_x(x^*) \times \mathcal{U}_C(C^*)$ be defined as above.*

Then there exists a neighborhood of C^ in \mathcal{C} , which we again denote by $\mathcal{U}_C(C^*)$ such that $H(y(C), \xi)$ is positive definite for all $C \in \mathcal{U}_C(C^*)$. Here, for given C and $x(C)$ the function $\xi \in Z$ denotes the unique solution of $e_x^*(y(C))\xi = -Q_x(y(C))$ in Z^* .*

Proof: It is sufficient to show that $H(y^*, \xi^*)$ is positive definite. Positive definiteness of $H(y(C), \xi)$ for all $C \in \mathcal{U}_C(C^*)$ with a suitably small neighborhood $\mathcal{U}_C(C^*)$ then follows from a continuity argument. Now set $x \stackrel{\text{def}}{=} e_x^{-1}(y^*)e_C(y^*)C$ for $C \in \mathcal{C}$. Similar arguments as in the proof of Theorem 3.3 yield directly

$$\langle H(y^*, \xi^*)C, C \rangle_{\mathcal{C}} \geq \gamma \|C\|_{\mathcal{C}}^2 - c \|x\|_X^2 \|\xi^*\|_Z \geq (-c \|Q_x(y^*)\|_{X^*} + \gamma) \|C\|_{\mathcal{C}}^2,$$

which gives the claim.

With these preparations we are in the position to prove the local quadratic convergence of Newton's method.

Theorem 4.2. *Let the assumptions of Theorem 3.3 be satisfied. Further, let $y^* = (x(C^*), C^*)$ denote a solution of problem (2.8) and let ξ^* be the associated Lagrange multiplier. Then there exists a neighborhood $\mathcal{U}(y^*) = \mathcal{U}_x(x^*) \times \mathcal{U}_C(C^*) \subset X \times \mathcal{C}$ such that for every starting point $C^0 \in \mathcal{U}_C(C^*)$ the Newton iterates $\{C^k\}_{k \in \mathbb{N}}$ remain in $\mathcal{U}_C(C^*)$ and converge quadratically to C^* . Furthermore, the corresponding states $x^k = x(C^k)$ remain in $\mathcal{U}_x(x^*)$ and converge to x^* .*

Proof: By Proposition 4.1 $H(y(C^*), \xi^*)$ is positive definite. Therefore, C^* is a local minimum of \hat{Q} . By a continuity argument a neighborhood $\mathcal{U}_C(C^*) \subset \mathcal{C}$ exists, such that $H(y(C), \xi)$ is Lipschitz continuous for all $C \in \mathcal{U}_C(C^*)$, where $\xi = \xi(C)$. Therefore the assumptions for both, the Newton-Mysovskii and the Newton-Kantorovitch Theorem [Deu04] are satisfied, so that the claim follows for the convergence of the Newton iterates $\{C^k\}_{k \in \mathbb{N}}$. Since the state x depends continuously on C this concludes the proof.

Remark 4.3. Assumptions **A.1–A.6** together with Theorem 3.3 now also imply local quadratic convergence of the basic SQP algorithm applied to problem 2.8. For details we refer to [HK01, IK96].

We are now in the position to formulate Newton's method for the numerical solution of equation $\hat{Q}'(C^*) = 0$, which is the first order necessary condition of problem (4.1), and to prove local quadratic convergence of the algorithm.

Algorithm 1. (Newton's algorithm)

Let $C^0 \in \mathcal{U}_C(C^*)$ be given.

- i) Set $k = 0$ and $C^0 = C_0$.
- ii) Do while the stopping criterion is violated
 - (1) Set $y^k = (x(C^k), C^k)$ and $\xi^k = -e_x^{-*}(y^k)Q_x(y^k)$
 - (2) Solve $H(y^k, \xi^k)\delta C^k = -\hat{Q}'(C^k)$
 - (3) Set $C^{k+1} = C^k + \delta C^k$, $k = k + 1$
- iii) $C^* \stackrel{\text{def}}{=} C^k$, $y^* \stackrel{\text{def}}{=} y^k$, STOP.

Remark 4.4. We note that due to the structure of the reduced Hessian the Newton system in step ii)(2) has to be solved iteratively. Let us refer to this as the inner iteration. To provide the right hand side in ii)(2) one has to solve the nonlinear equation $e(x^k, C^k) = 0$ in Z^* for $x^k \in X$, and one needs to solve the adjoint equation $\xi^k = -e_x^{-*}(y^k)Q_x(y^k)$. These are all ingredients for the calculation of \hat{Q}' from (4.2).

Every application of $H(y^k, \xi^k)$ in the j -th inner iteration amounts to two linear solves, namely

$$v_j^k = e_x^{-1}(y^k)e_C(y^k)\delta C_j^k$$

and

$$w_j^k = e_C^*(y^k)e_x^{-*}(y^k) \{Q_{xx}(y^k) + \langle e_{xx}(y^k)(v_j^k, v_j^k), \xi \rangle_{Z^*, Z}\}.$$

We give now the precise systems of linear equations which have to be solved for the evaluation of the Hessian. For the computation of $v_j^k = (v^{J_n}, v^{J_p}, v^n, v^p, v^V)$ one needs in fact

to solve the linear system

$$v^{J_n} - (\nabla v^n + v^n \nabla V + n \nabla v^V) = 0, \quad (4.4a)$$

$$v^{J_p} + (\nabla v^p - v^p \nabla V - p \nabla v^V) = 0, \quad (4.4b)$$

$$\operatorname{div} v^{J_n} - R_n v^n - R_p v^p = 0, \quad (4.4c)$$

$$\operatorname{div} v^{J_p} + R_n v^n + R_p v^p = 0, \quad (4.4d)$$

$$-\lambda^2 \Delta v^V - v^n + v^p = \delta C_j^k, \quad (4.4e)$$

supplemented with homogeneous Dirichlet and Neumann data along Γ_D and Γ_N , respectively.

Remark 4.5. Again, two variables can be eliminated using the first two equations, which yields the system

$$\begin{aligned} \operatorname{div} (\nabla v^n + v^n \nabla V + n \nabla v^V) &= R_n v^n + R_p v^p, \\ \operatorname{div} (\nabla v^p - v^p \nabla V - p \nabla v^V) &= R_n v^n + R_p v^p, \\ -\lambda^2 \Delta v^V - v^n + v^p &= \delta C_j^k. \end{aligned}$$

Further, for the computation of $w_j^k = (w^{J_n}, w^{J_p}, w^n, w^p, w^V)$ one needs to solve the linear system

$$w^n = \nabla w^{J_n}, \quad (4.5a)$$

$$w^p = \nabla w^{J_p}, \quad (4.5b)$$

$$\operatorname{div} w^n - w^n \nabla V = w^V + R_n w^{J_n} - R_n w^{J_p} + \nabla v^V \xi^n + (R_{nn} v^n + R_{np} v^p)(\xi^{J_p} - \xi^{J_n}), \quad (4.5c)$$

$$\operatorname{div} w^p + w^p \nabla V = w^V - R_p w^{J_n} + R_p w^{J_p} - \nabla v^V \xi^p + (R_{np} v^n + R_{pp} v^p)(\xi^{J_p} - \xi^{J_n}), \quad (4.5d)$$

$$-\lambda^2 \Delta w^V + \operatorname{div}(n w^n) + \operatorname{div}(p w^p) = -\operatorname{div}(v^n \xi^n) + \operatorname{div}(v^p \xi^p), \quad (4.5e)$$

supplemented with the following set of boundary conditions

$$w^{J_n} = \begin{cases} v^n, & \text{on } \Gamma_O, \\ 0, & \text{on } \Gamma_D \setminus \Gamma_O, \end{cases} \quad (4.5f)$$

$$w^{J_p} = \begin{cases} -v^p, & \text{on } \Gamma_O, \\ 0, & \text{on } \Gamma_D \setminus \Gamma_O, \end{cases} \quad (4.5g)$$

$$w^V = 0, \quad \text{on } \Gamma_D, \quad (4.5h)$$

as well as

$$w^n \cdot \nu = w^p \cdot \nu = \nabla w^V \cdot \nu = 0 \quad \text{on } \Gamma_N. \quad (4.5i)$$

Remark 4.6. Also in this system two variables can be eliminated using the first two equations, which yields the system

$$\begin{aligned}\Delta w^{J_n} - \nabla w^{J_n} \nabla V &= w^V + R_n w^{J_n} - R_n w^{J_p} + \nabla v^V \xi^n + (R_{nn} v^n + R_{np} v^p)(\xi^{J_p} - \xi^{J_n}), \\ \Delta w^{J_p} + \nabla w^{J_p} \nabla V &= w^V - R_p w^{J_n} + R_p w^{J_p} - \nabla v^V \xi^p + (R_{np} v^n + R_{pp} v^p)(\xi^{J_p} - \xi^{J_n}), \\ -\lambda^2 \Delta w^V + \operatorname{div}(n \nabla w^{J_n}) + \operatorname{div}(p \nabla w^{J_p}) &= -\operatorname{div}(v^n \xi^n) + \operatorname{div}(v^p \xi^p).\end{aligned}$$

Finally, we state the desired algorithm.

Algorithm 2. (Newton's method with inner iteration)

1. Choose C^0 in a neighborhood of C^* .
2. For $k = 0, 1, 2, \dots$
 - (a) Evaluate $\hat{Q}'(C^k)$, choose δC_0^k and set $j = 0$.
 - (b) Solve step ii)(2) of Algorithm 1 iteratively:
$$\delta C^k = \operatorname{Iteration}(H(y^k, \xi^k), \delta C_0^k, j)$$
 - (c) Set $C^{k+1} = C^k + \delta C^k$

5 Numerical Results

In this section we want to study the numerical performance of Algorithm 2. We apply the algorithm for the optimization of an unsymmetric n–p–diode, whose reference doping profile \bar{C} can be found in Figure 5.1. For the computations we chose the following nondimensional parameters for the state system (1.2):

$$\lambda^2 = 10^{-3}, \quad \delta^2 = 10^{-2}, \quad U = 10,$$

which are typical for standard devices. The computations were performed on a uniform one dimensional grid with 1000 points and the state system was discretized using the well-known Scharfetter–Gummel discretization [SG69], which is essentially an exponentially fitted scheme allowing for the resolution of the steep gradients near to the junction [GMS98, BMP89]. Also for the adjoint system (3.3) and the linearized state system (4.4) we used an adapted Scharfetter–Gummel discretization [BP]. This is essential to ensure the convergence of the inner loop in the Newton algorithm.

Remark 5.1. In general, we cannot expect the global convergence of Newton's method far away from the minimizer. Hence, we require an additional globalization strategy to ensure its convergence, owing to the fact that we only have local convexity near to the minimizer. There are good strategies at hand (ranging from a standard damped Newton's method [Kel95] to sophisticated trust–region modifications that can be implemented using Steihaug's variant of the CG algorithm, cf. [Ste83, Kel99]). Thus, we shall not go into further details.

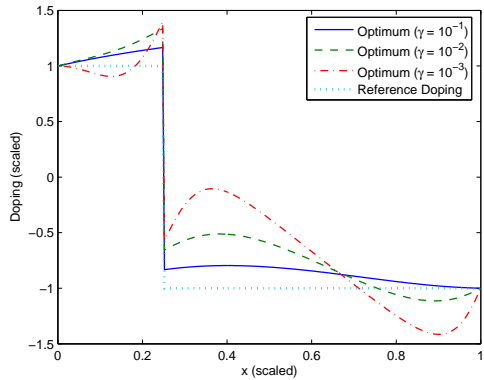


Figure 5.1: Dependence of the optimum on γ

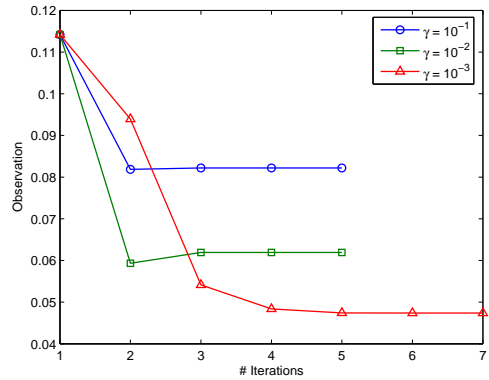


Figure 5.2: Dependence of the observation on γ

5.1 Influence of the Regularization Parameter γ

First, we tried to achieve an increase of the electron and hole current by 50 % and studied the influence of the regularization parameter γ . The different resulting optimal doping profiles can be found in Figure 5.1. As expected we get larger deviations from \bar{C} for decreasing γ , which on the other hand also allows for a better reduction of the observation as can be seen in Figure 5.2. For all three cases we already get a significant reduction after two steps and the algorithm terminates rather quickly. Only for the smallest value of γ we need two more iterations to meet the stopping criterion, which can be explained by a loss of convexity or, equivalently, a weaker definiteness of the Hessian.

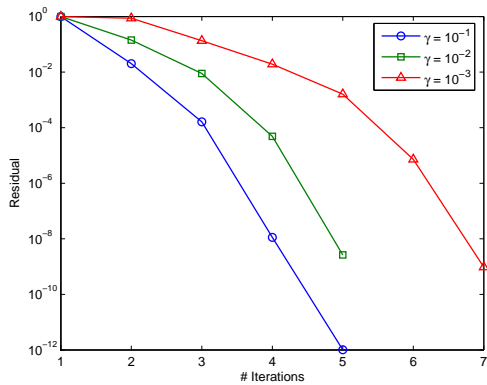


Figure 5.3: Dependence of the residual on γ

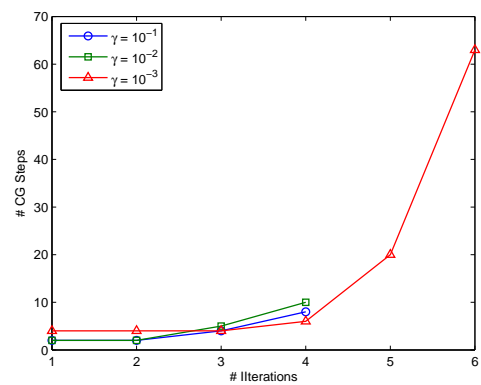


Figure 5.4: Dependence of the CG iteration on γ

The conjugate gradient algorithm in the inner loop was terminated when the norm of the gradient became sufficiently small; to be more precise, in the j -th conjugate gradient step

for the computation of the update in Newton step k we stop if the residual r_j^k satisfies

$$\frac{\|r_j^k\|}{\|\hat{Q}'(C^0)\|} \leq \min \left\{ \left(\frac{\|\hat{Q}'(C^k)\|}{\|\hat{Q}'(C^0)\|} \right)^q, p \frac{\|\hat{Q}'(C^k)\|}{\|\hat{Q}'(C^0)\|} \right\} \quad \text{or} \quad j \geq 100. \quad (5.1)$$

Note, that $q \in (1, 2)$ determines the convergence order of the outer Newton algorithm. The value of $p \in (0, 1)$ is important for the first step of Newton's method, as for $k = 0$ the norm quotients are all 1; for later steps, the influence of q becomes increasingly dominant.

To get deeper insight into the convergence behavior of the algorithm, we present in Figure 5.3 the norm of the residual during the iteration for different values of γ . Here, we used $q = 2$ to get the desired quadratic convergence behavior. Again, one realizes that the convergence deteriorates with decreasing γ . Since the overall numerical effort is spent in the inner loop, we show the number of conjugate gradient steps in Figure 5.4. Here, one realizes the drastic influence of the regularization parameter.

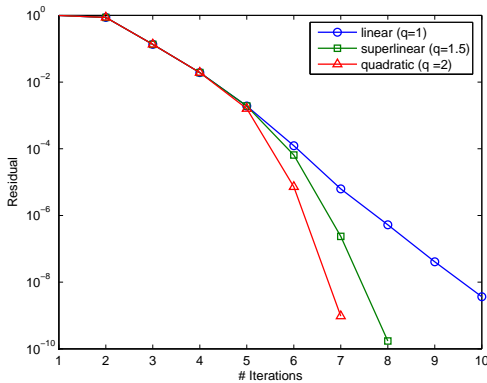


Figure 5.5: Dependence of the residual on q

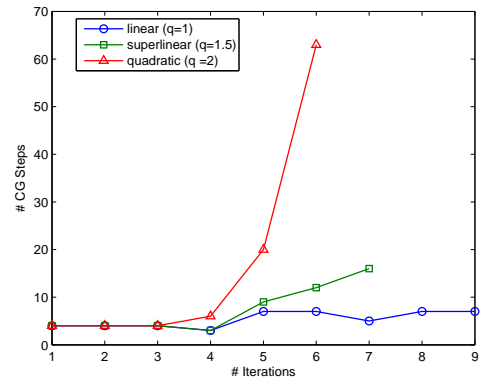


Figure 5.6: Dependence of the CG iteration on q

5.2 Influence of the Stopping Criterion

The next numerical test was devoted to the stopping criterion of the inner iteration and the influence of the exponent q . In Figure 5.5 the decrease of the residual is depicted for different values of $q = 1, 1.5, \text{ or } 2$. As predicted by the general theory [Kel95] one gets linear, superlinear and quadratic convergence. Clearly, the parameter q strongly influences the number of conjugate gradient steps, which can be seen from Figure 5.6. While in the linear case ($q = 1$) we have an almost constant amount of CG steps in each each iteration, we get, as expected, a drastic increase towards the end of the iteration for the quadratic case ($q = 2$). Hence, the overall numerical effort in terms of CG steps is despite of the quadratic convergence much larger compared to the relaxed stopping criterion, which only yields linear convergence!

5.3 Influence of the Grid Size

Finally, we study the performance of Algorithm 2 with respect to the grid spacing h . We keep the stopping criterion and the regularization parameter fixed and just vary the grid size h from $1/500$ over $1/1000$ down to $1/2000$. The evolution of the residual for these three cases is depicted in Figure 5.7. The numerical results suggest that the algorithm is grid independent, which is essential for large scale optimization purposes. Nevertheless, there is a negligible dependence of the number of CG iterations on the grid spacing as can be seen from Figure 5.8.

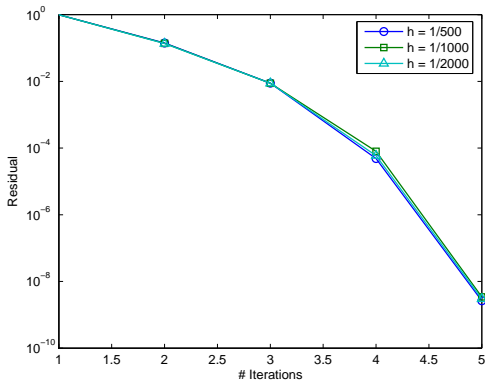


Figure 5.7: Dependence of the residual on the grid

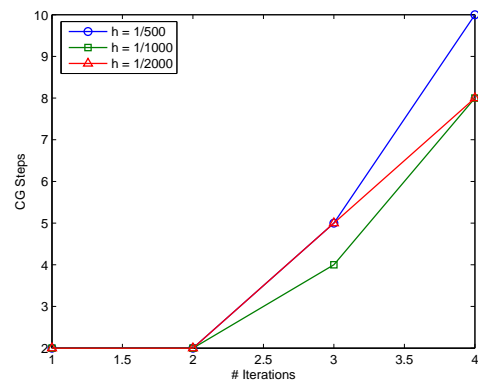


Figure 5.8: Dependence of the CG iteration on the grid

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