

# Inverse Doping Profile Analysis for Semiconductor Quality Control

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Dissertation Abstract

PhD awarded December 12, 2009, Wichita State University

## 1 Preface

Today we live in an incredible computer age. Barely more than 50 years ago—an imperceptible drop in the ocean of history’s timescale—the state-of-the-art SAGE United States national air-defense computer network [6] consisted of 55,000 vacuum tubes powered by three megawatts of electricity and housed in facilities totaling almost two acres in size. A tiny microprocessor today contains an electric circuit so sophisticated and complicated that it contains 40,000 times as many components, each one of which processes much larger chunks of data than a component in the SAGE air-defense computer network. If the latest computer processors today were constructed using the same technology as the SAGE air-defense network, they would consume more than 12 times as much power as the entire city of New York. Yet today the same computing capability can be produced using less power than a 100-watt light bulb!

The way that circuits so complicated can be created so small is by an incredible “printing” process.<sup>1</sup> Instead of printing ink *onto* paper, a special apparatus (Figure 1) precisely imprints an invisible electric circuit *into* a solid substrate made of silicon or another semiconductor. The doping apparatus is designed to use heat and pressure to forcibly add impurities to selected areas of the semiconductor. Even tiny concentrations of impurities can change the electric conductivity by factors much greater than 10,000, creating the equivalent of copper wires on a microscopic scale, each “wire“ being less than 65 nanometers thick (many times smaller than the wavelength of blue light).

The “printing” process is called “doping,” and the resulting invisible electric circuit is called the “doping profile.” As we read on, we will see how the goal of perceiving or deducing something which is ordinarily invisible, by mathematical methods, is called solving an **inverse problem**. Identification of the doping profile by mathematical methods permits reverse engineering of the electric circuit characteristics, and thus the properties, performance, and functionality of the semiconductor device, to achieve the goal of quality control.

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<sup>1</sup>In reality, the fabrication of computer chips is much more complicated than this simplified explanation.

## 2 Introduction

Both our lives and lifestyles daily depend on a host of invisible semiconductor devices, whose functionality or failure often means life or death. If for some reason the doping compounds fail to be imprinted properly, one is faced with the failure of a semiconductor device—nothing less than an absolute nightmare—and the necessity of improved quality control is unbelievably emphasized. As an example, graphics giant NVIDIA lost \$200 million recently because of one set of defective chipsets, and there were several articles suggesting that a temperature offset within the foundry of as little as four degrees Celsius was responsible; as a result, NVIDIA endured a drop in stock price from \$39.67 to \$5.75, as well as losing substantial market share to rival ATI. The problem could possibly have been circumvented by advances in quality control.

One's goal is to achieve quality control in the manufacture of semiconductor devices, i.e., the microscopic components and subcomponents of the electric circuits embedded through “doping profile” methods on a “computer chip.” P-N junctions are used to form multiple types of transistors—these are fundamental building blocks of an incredible array of semiconductor devices—on which a modern world is built: health care, medical applications, computers, cell phones, navigational systems, and the Internet.

Currently, however, only destructive techniques, like spreading resistance profiling, are easily available for quality control purposes. There are three stepping stones towards ultimate success in implementing non-destructive, efficient quality control methods for semiconductor manufacturing. These are to

1. Find, develop, and use the mathematical framework underlying the semiconductor quality control problem, including a precise mathematical definition of the semiconductor doping profile as a function  $C$  specifying the signed difference between concentrations of positive and negative charge carriers (holes and electrons).
2. Create an efficient numerical algorithm for finding as much information about  $C$  as possible from the smallest amount of data measurements available.
3. Fine-tune the numerical algorithm to real-world manufacturing data and real-time manufacturing environments, enabling one to realize the final goal of producing extremely reliable semiconductor devices.

The first two goals are largely accomplished within the dissertation, with a great deal of help from results available in the mathematical literature, especially the topics of conformal mapping and identification of coefficients in some semilinear elliptic boundary value problems.

In Step 2, we consider the suggested numerical algorithm to be one of the most significant contributions in the dissertation towards the final goal of quality control in the setting of industrial manufacture of semiconductor devices. The numerical algorithm will solve many “direct” problems in order to ultimately converge to the solution of the “inverse” problem. In the creation of the numerical algorithm, simulations are extremely important, where the speed

of the computer code can be tested and refined. One finds that execution speed can be reduced from over one minute for a single solution of the direct problem on a 50-by-50 grid, to less than one hundredth of a second on a 100-by-100 grid, by using advanced integral equation techniques and methods of complex variables.

The result is an algorithm which can perform solution of the inverse problem from 1/3rd of a second up to 10 seconds (30 to 1,000 iterations) with four times as much accuracy, compared to an algorithm which would take from half an hour to almost one full day and night, with four times less accuracy. Clearly these optimizations make a difference in the suitability of the algorithm for practical use, which, to use a parallel to the previous sentence, is just as big of a difference as the difference between night and day.

Beyond the first two steps, the final step of going beyond computer simulations to actual physical implementation is yet to be carried out, and it will need collaboration between—at minimum—electrical engineers, semiconductor physicists, and applied mathematicians.

### 3 Mathematical framework

One may look at the great timeline of history and shall find that every time scientists reached a greater understanding of the mathematical principles governing an unknown area of electromagnetics, physics, or physical chemistry, that almost without fail there would immediately follow great accomplishments, discoveries, and forward momentum in the development, growth, blossoming, and maturation towards the present age of computers. Mathematics has practical applications which far exceed the mere ability to solve esoteric puzzles—when a problem whose origin is reality has been framed in representative mathematical terms, and when someone has then solved the mathematical problem associated with reality, then one has the best chance, sometimes the only chance, to solve the problem that exists, as one would say, “in the real world.” In the classical sense of Hadamard, this is the idea of a “Well-Posed Mathematical Inverse Problem.” But the general meaning of an “Inverse Problem” is to identify a set of  $x$ -values based on some knowledge about the functional relationship  $f(x) = y$  (“some knowledge” often corresponds to partial differential or integral equations satisfied by  $x$  and  $y$ ) and some other additional, more specific and direct, knowledge about  $y$ . The idea of such a generalized inverse problem can be summarized by trying to identify the criminal(s)  $x$  by the results of their crime  $f(x)$ . One cannot “see inside” of the function  $f$ , which represents the “past” or a “forbidden region,” and so the mathematical analyst (the police detective) must deduce the identity of  $x$  (the criminal) by more or less indirect methods. For instance, if we wish to identify the doping profile of a semiconductor device without destroying it, then the semiconductor wafer is a “forbidden region,” containing a region of altered electrical properties formed by addition of doping materials to the base semiconductor substrate. This “doped” region is the unknown “ $x$ .”

The famous detective, Sherlock Holmes, in trying to explain his detective work, provides us with an excellent

Table 1: History of the inverse doping problem

1947	The invention of an effective “transistor” takes place.
1950	Roosbroeck develops the drift-diffusion equations for doping profiles.
1953	Transistors become successful building blocks for many devices.
1980	Calderón brings attention to the inverse problem for conductivity.

literary viewpoint of inverse problems:

*“Most people, if you describe a train of events to them will tell you what the result would be. They can put those events together in their minds, and argue from them that something will come to pass. There are few people, however, who, if you told them a result, would be able to evolve from their own inner consciousness what the steps were which led up to that result. This power is what I mean when I talk of reasoning backward, or analytically.”*

— **A Study in Scarlet**, Sir Arthur Conan Doyle

To find the unknown “x,” we must rely on the mathematical framework that defines “x.” This is the system of drift-diffusion equations.

Our starting point for mathematical analysis is a commonly accepted model of the semiconductor device, the *drift diffusion equations* [8]. We note that this system of equations is quite similar in its properties to the equations from Combustion Theory [1, Ch. 2]. Although the most widely accepted model for semiconductor devices, the drift diffusion equations already represent a compromise that is made between the ideal of accurately describing the underlying device physics, and the feasibility of computational solutions for the chosen nonlinear system of partial differential equations.

We consider the following coupled system [10] of nonlinear partial differential equations for electrostatic potential  $V$ , the nonnegative concentrations of free carriers of negative charge density  $n$  (electrons) and positive charge density  $p$  (holes), which is solved in the domain  $\Omega \subset \mathbb{R}^d (d = 1, 2, 3)$  representing the semiconductor device, and in a time interval  $[0, T]$ . The dependence on time that is included in this system of equations should be emphasized.

$$\begin{aligned}
 \operatorname{div}(\epsilon_s \nabla V) &= q(n - p - C), \\
 \operatorname{div}(D_n(E, T^K) \nabla n - \mu_n(E, T^K) n \nabla V) &= n_t, \\
 \operatorname{div}(D_p(E, T^K) \nabla p + \mu_p(E, T^K) p \nabla V) &= p_t, \\
 \operatorname{div} k(T^K) \nabla (T^K) &= \rho c(T^K) T_t^K - H.
 \end{aligned} \tag{1}$$

Above  $\epsilon_s$  denotes the positive semiconductor permittivity coefficient (e.g., for silicon) and  $q$  the positive unit of elementary charge—both  $\epsilon_s$  and  $q$  depend on dimension;  $\mu_n$  and  $\mu_p$  denote the electron and hole mobility, and  $D_n$  and  $D_p$  are the electron and hole diffusion coefficients. Observe that  $-\nabla V$  is the electric field with electric field strength  $E = |\nabla V|$ . The function  $R = R(n, p, x)$  denotes the recombination-generation rate.

The constants  $\rho$  and  $c$  represent the specific mass density and specific heat of the material. In the thermodynamic

description,  $k$  and  $H$  denote the thermal conductivity and the locally generated heat.  $T^K$  is the absolute temperature.

We assume that  $R$  is of the standard form

$$R = F(n, p, x)(np - n_i^2), \quad (2)$$

where  $F$  is a nonnegative smooth function, which holds, for example, for the frequently used *Shockley-Read-Hall* rate

$$R_{SRH} = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)}. \quad (3)$$

The function  $C = C(x)$  represents the doping concentration, which is produced by diffusion of different materials into the silicon crystal (zone melting technique) and by implantation with an ion beam. When  $C < 0$  it represents the P region of the semiconductor and when  $C > 0$  it represents the N region. See the literature [3, 7, 2, 8, 11] for more details. [Note that there is a mistake in [4], which specifies on page 1,778 that  $C > 0$  in both P and N regions.]

This system is supplemented by homogeneous Neumann boundary conditions on an insulated part  $\partial\Omega_N$  (open in  $\partial\Omega$  of the boundary, where zero current flow and zero electric field in the normal direction are prescribed [9]). On the remaining part  $\partial\Omega_D$  (with positive  $(d-1)$ -dimensional Lebesgue measure), the following Dirichlet conditions are imposed:

$$V(x, t) = V_D(x, t) = U(x, t) + V_{bi}(x) = U(x) + U_T \ln \left( \frac{n_D(x)}{n_i} \right), \quad (4)$$

$$n(x, t) = n_D(x) = \frac{1}{2} \left( C(x) + \sqrt{(C(x))^2 + 4n_i^2} \right), \quad (5)$$

$$p(x, t) = p_D(x) = \frac{1}{2} \left( \sqrt{(C(x))^2 + 4n_i^2} - C(x) \right), \quad (6)$$

on  $\partial\Omega_D \times (0, T)$ , where  $n_i$  is the intrinsic carrier density,  $U_T$  is the (nonnegative) thermal voltage and  $U$  is the applied potential. Moreover, the initial (time) conditions,

$$\begin{aligned} n(x, 0) &= n_0(x) \geq 0, \\ p(x, 0) &= p_0(x) \geq 0. \end{aligned} \quad (7)$$

have to be supplied.

## 4 Stationary drift-diffusion equations

The *stationary drift-diffusion model* is obtained from the transient model by suppressing time-dependence and omitting the initial (time) conditions. We use standard assumptions about the mobilities and diffusion coefficients

(Einstein relations),

$$\begin{aligned} D_n &= \mu_n U_T, \\ D_p &= \mu_p U_T, \end{aligned} \tag{8}$$

in order to transform the system using the so-called *Slotboom variables*  $u$  and  $v$  defined by

$$\begin{aligned} n &= C_0 \delta^2 e^{V/U_T} u, \\ p &= C_0 \delta^2 e^{-V/U_T} v, \end{aligned} \tag{9}$$

where

$$\delta^2 = \frac{n_i}{C_0}, \tag{10}$$

and  $C_0$  is the doping profile scale. If we rescale all quantities to dimensionless analogues (see [8] for further details), and if we define scaled current densities for electrons and holes,

$$\begin{aligned} J_n &= \mu_n \delta^2 e^V \nabla u, \\ J_p &= \mu_p \delta^2 e^{-V} \nabla v, \end{aligned} \tag{11}$$

then we obtain the stationary system

$$\begin{aligned} \lambda^2 \Delta V &= \delta^2 (e^V u - e^{-V} v) - C, \\ \operatorname{div} J_n &= \delta^4 Q(u, v, V, x)(uv - 1), \\ \operatorname{div} J_p &= -\delta^4 Q(u, v, V, x)(uv - 1). \end{aligned} \tag{12}$$

Above  $\lambda^2$  is a positive constant,

$$\lambda^2 = \frac{\epsilon_s U_T}{q C_0 L^2}, \tag{13}$$

where  $L$  is a typical length scale of a semiconductor device, usually about  $10^{-4}$  cm. In order to obtain a completely non-dimensional system, we have used the scaled length  $x/L$ , and replaced the mobilities  $\mu_n$  and  $\mu_p$  by  $(U_T/L)\mu_n$  and  $(U_T/L)\mu_p$ . We have also assumed  $\epsilon_s$  is constant and rescaled the potential to  $V/U_T$ . Also,  $Q$  is defined by the relation  $F(n, p, x) = Q(u, v, V, x)$ .

The Dirichlet boundary conditions can be written as

$$V = U + V_{bi} = U + \ln \left( \frac{1}{2\delta^2} (C + \sqrt{C^2 + 4\delta^2}) \right) \text{ on } \partial\Omega_D, \tag{14}$$

Table 2: Meanings of drift diffusion symbols

$\epsilon_s$	semiconductor permittivity
$q$	elementary charge
$\mu_n$	electron mobility
$\mu_p$	hole mobility
$D_n$	electron diffusion coefficient
$D_p$	hole diffusion coefficient
$R$	recombination-regeneration rate (in general depends on $n, p$ )

and

$$\begin{aligned} u &= e^{-U} && \text{on } \partial\Omega_D, \\ v &= e^U && \text{on } \partial\Omega_D. \end{aligned} \tag{15}$$

On the remaining part  $\partial\Omega_N = \partial\Omega \setminus \partial\Omega_D$ , the homogeneous Neumann conditions can be formulated in terms of  $J_n$  and  $J_p$ , i.e.,

$$\left. \begin{aligned} \partial_\nu V &= \partial_\nu J_n, \\ \partial_\nu J_n &= \partial_\nu J_p, \\ \partial_\nu J_p &= 0, \end{aligned} \right\} \text{on } \partial\Omega_N. \tag{16}$$

Complete understanding is lacking even for this system of elliptic parabolic quasilinear equations. Depending on the type of information desired about the semiconductor device, it is necessary to isolate a certain subset of the difficult problems which solid-state physics poses to the mathematician. Due to the partial electrical resemblance between the P-N junction and an inductor or capacitor, it is doubtful that extremely detailed information about  $C(x)$ , the doping profile, can be determined from inverse problems neglecting the time dependence of the equations, since inductance and capacitance are both effects which involve time. However, an amazing amount of analysis can still be done using only voltage and current measurements, which assume only a steady-state equilibrium.

To continue the analysis, the dissertation linearizes the solution around an equilibrium state, then formulates an ‘‘adjoint’’ inverse problem to simplify boundary data for numerical analysis. This approach is widely used in the inverse option pricing problem (Dupire’s equation) [5]. We apply the results to the case when a vertical profile of the semiconductor device is scanned with boundary measurements of voltage and current. One must analyze these measurements and reconstruct the doping profile in the interior of the given two-dimensional domain. By concatenating the two-dimensional images which are generated, one may reconstruct the unknown three-dimensional object.

## 5 Theoretical uniqueness results

Stability of a computational algorithm, such as one for reconstruction of an unknown function like the doping profile, depends primarily on uniqueness of the desired unknown within a suitable class of functions. It is extremely

important to determine the extent of this function class, and to use this knowledge in creation of the computational algorithm for determining the unknown function. Hence, some of the most critical components of the dissertation are its theoretical uniqueness results, which can be applied not only to problems in doping profile theory, but also to similar mathematical problems, such as ion channels in inter-cellular transport. Although the uniqueness results take up 27 pages in the original document, they can be summarized briefly in a few sentences, as follows.

Global uniqueness for a doping profile, even a discontinuous one, is proved in the case of many boundary measurements (Dirichlet-to-Neumann map) by linearizing the partial differential equations around the solution with zero boundary data, and using known results about determination of unknown coefficients by the Dirichlet-to-Neumann map. Using a proof by contradiction, it is also proved that local uniqueness for the same class of doping profiles holds in the case of one boundary measurement; the proof also uses results of geometric critical points and conformal mapping index theory. Moreover, global uniqueness of a doping profile is proved in the case when  $\Omega$  is the union of sets  $P = \{x : C(x) = a\}$  and  $\{x : C(x) = b\}$  for constants  $a \neq b$ , and when  $P$  is a convex polygon.

## 6 Computational algorithm

We propose to identify the area, shape, and location of the obstacle  $D$  by using a three-step algorithm.

1. Generate initial data for inverse problem.
  - (a) Impose potential  $u = u_D$  on  $\Gamma_0$ .
  - (b) Measure the initial data for the inverse problem  $\partial_\nu u = u_N$  on  $\Gamma_0$ .
2. Compute the area and radius of  $D$ .
  - (a) Create artificial obstacle  $D_r$  which is circular and has radius equal to  $r$ .
  - (b) Solve the direct problem with obstacle  $D_r$  and the same potential  $u(;r) = u_D$  on  $\Gamma_0$  and find the resulting function  $\partial_\nu u(;r) = u_N(;r)$  on  $\Gamma_0$ .
  - (c) Find the radius  $r$  that minimizes  $\|u_N(;r) - u_N\|$ . (Here the norm  $\|\cdot\|$  is in  $L_\infty$  or another norm which works well in actual numerical experiments.)
  - (d) Fix this value of  $r$  and the area  $\pi r^2$  of the obstacle  $D_r$ .
3. Find the exact boundary of  $D$  by using perturbations which preserve the computed area of  $D$ .
  - (a) Represent  $D$  as deformations of the first approximation  $D_r$  ( $r$  is fixed, resulting from the previous step of the algorithm).
  - (b) Use a orthogonal coordinate system for the boundary of  $D$ .

$$\partial D := \gamma := \{ \langle x, y \rangle : \langle x, y \rangle = (r + h(s)) \langle \sin(s), \cos(s) \rangle \} \quad (17)$$

- (c) The first approximation  $h(s) = 0$  corresponds to  $D_r$ .
- (d) For better approximations take  $h(s)$  as a linear combination of basis functions such as sines and cosines

$$h(s) = \sum_{k=-n}^n (a_k \sin(kx) + b_k \cos(kx)) := a \cdot B_{\sin} + b \cdot B_{\cos}, \quad (18)$$

where  $a = (a_{-n}, a_{-n+1}, \dots, a_{n-1}, a_n)$  and  $b$  are multindexes. Write  $\alpha = (a, b)$  as a combined multindex.



- (e) Let  $\partial_\nu u(\cdot; \alpha) = u_N(\cdot; \alpha)$  on  $\Gamma_0$  be the data resulting from using the artificial domain  $D_\alpha$  with boundary  $\gamma(\alpha)$ .
- (f) Minimize  $\|u_N(\cdot; \alpha) - u_N\|$  with respect to  $\alpha$  to obtain an  $n$ -th order approximation  $D_\alpha$  of the domain  $D$ .

Figure 3 shows a peanut shaped domain (blue line) reconstructed (blue circles) successfully from measurements with  $\pm 5$  percent added random noise. The results shown are typical for any similar domain configuration.

## 7 Results

Our doping profile identification method has three primary benefits over existing methods for identifying conductivity or doping profiles. The necessary boundary measurements are very simple. The resolution is higher than results we have seen in the literature at the same level of noise. The type of measurements necessary are non-destructive to the semiconductor device. It should be made clear that we have only performed computer simulations with our method, and it has not been implemented or tested in industry.

Figures 4-13 show our method in action.

## 8 Industrial implementation—the step into the future

All of this mathematical and computational preparation serves only one purpose—to pose a question to researchers the world over, “Who is going to step to the plate and work as a team to achieve the final goal of reliable, efficient, and cost-effective quality control of semiconductor device manufacturing, based on the mathematical solution of the inverse doping profile problem?”

Similar problems of scientific research have been posed and solved at many critical times in world history. Examples include X-ray tomography (based on the Radon Transform, none other than the mathematical solution of an inverse problem), MRI and CAT scans, and many more fabulous, life-changing breakthroughs of science.

However, history also includes many problems that were never solved, not because it was impossible, but because not enough people worked together, not enough were willing to build on the results of one another. In order to achieve the goal of major improvements in semiconductor quality control, it is likely that much more work remains than what has already been done. Is the future bright for semiconductor quality control? The answer depends on the teamwork of many scientists—perhaps including you.

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## 9 Appendix: Figures

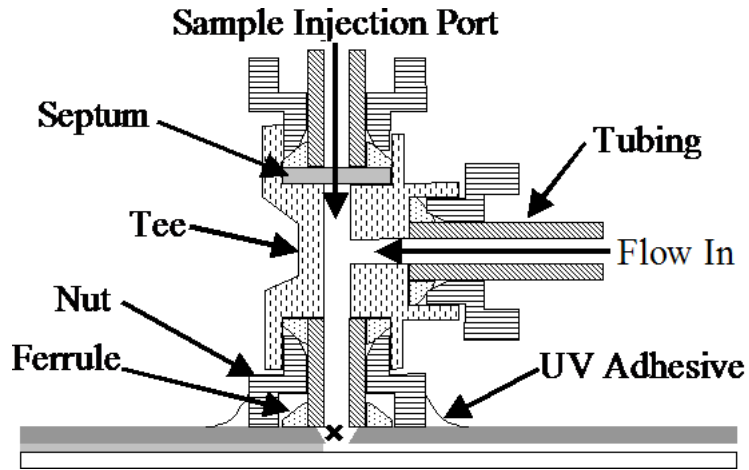


Figure 1: Apparatus used for doping of semiconductor devices

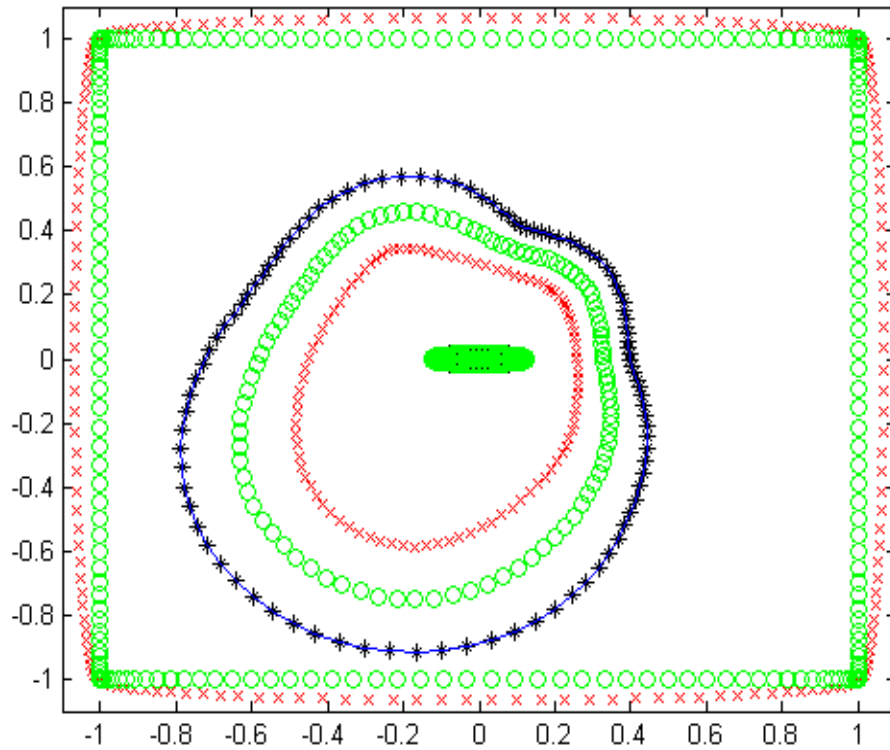


Figure 2: Optimized positioning of sources for curves of integration as generated by the dissertation's software package for Matlab

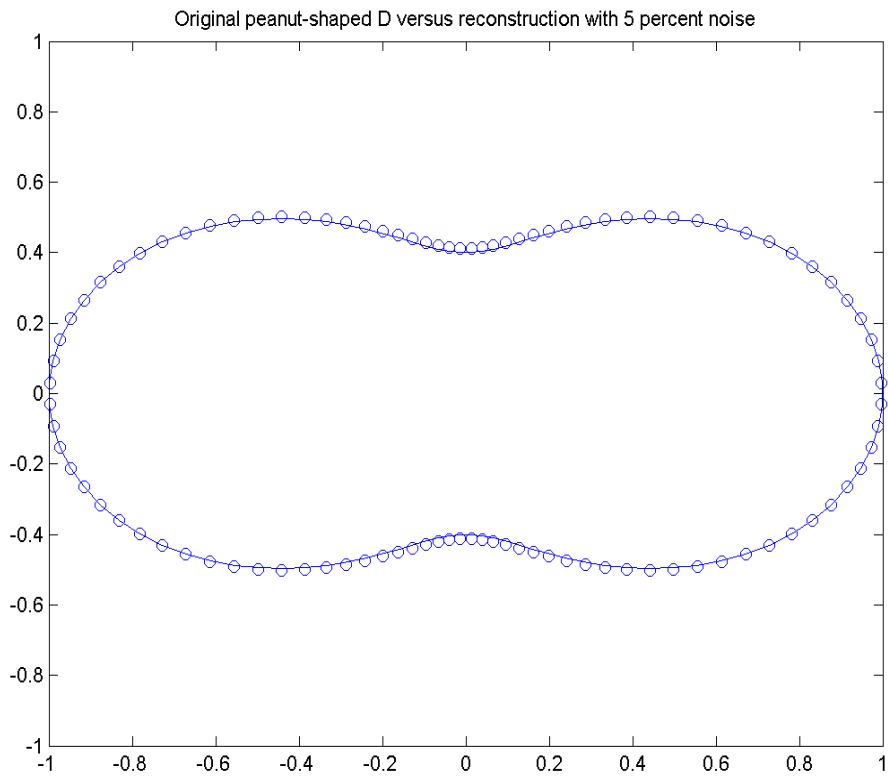


Figure 3: Good reconstruction of a peanut-shaped domain from data with 5 percent relative noise

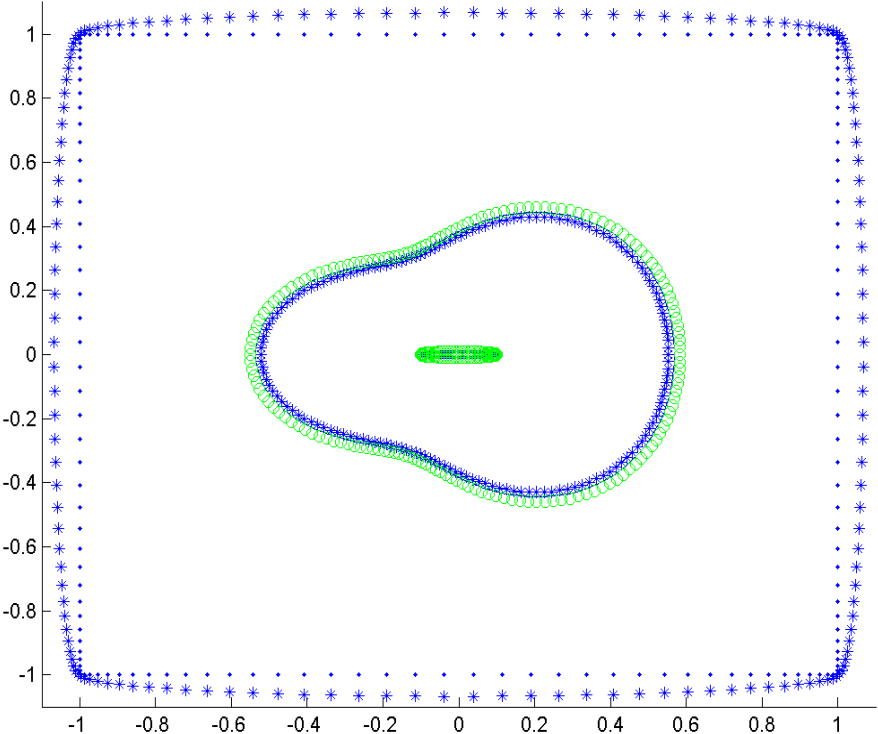


Figure 4: The curves of integration created automatically by a subroutine we wrote as part of a Matlab package for solving inverse conductivity problems by integral equation methods.

### Inner/Outer Direct Problem Solutions

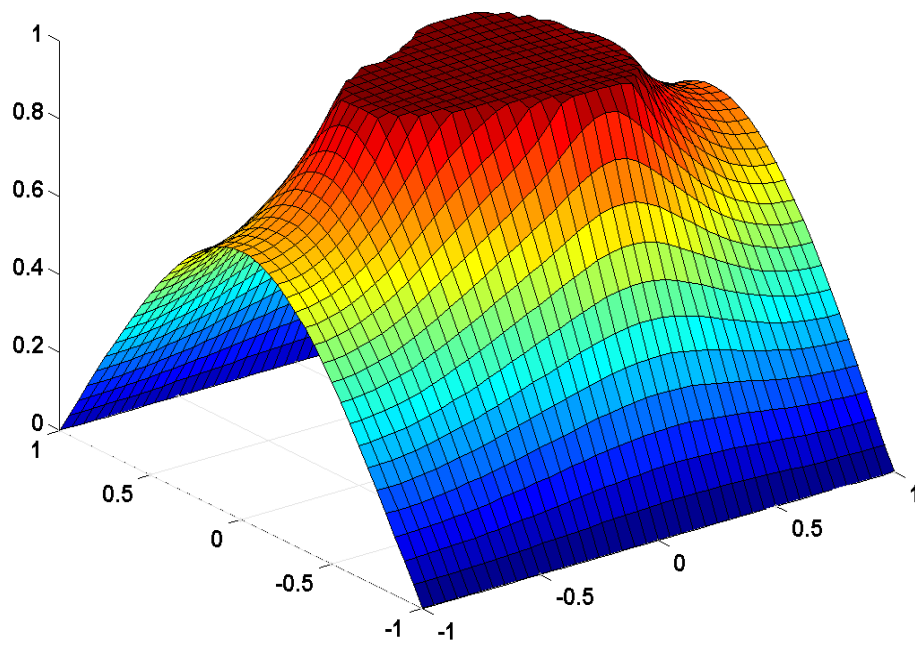


Figure 5: The potential surface.

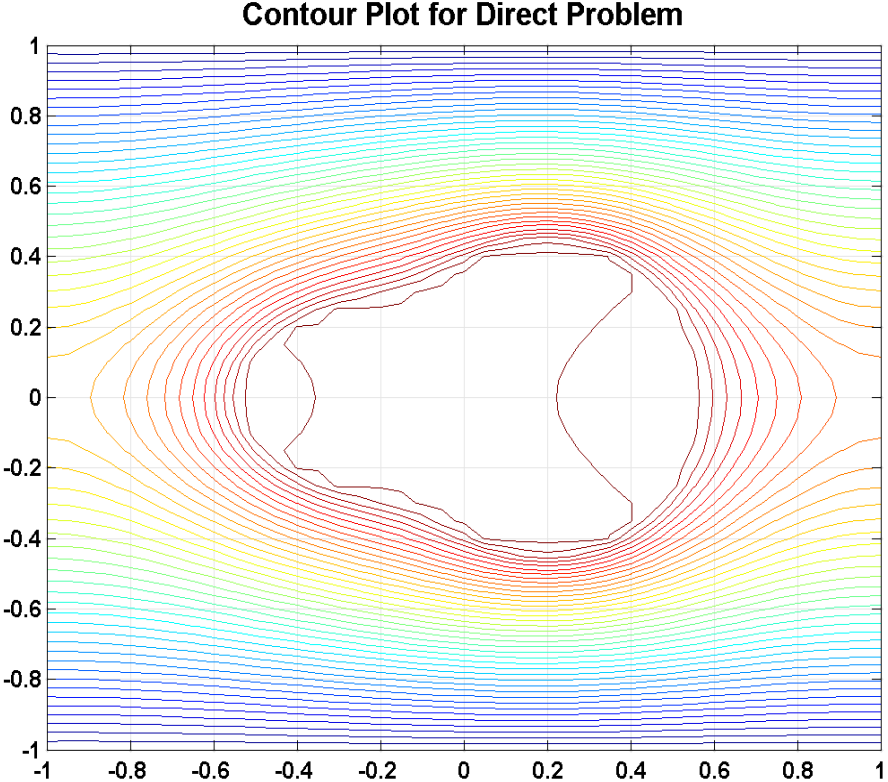


Figure 6: The level curves.



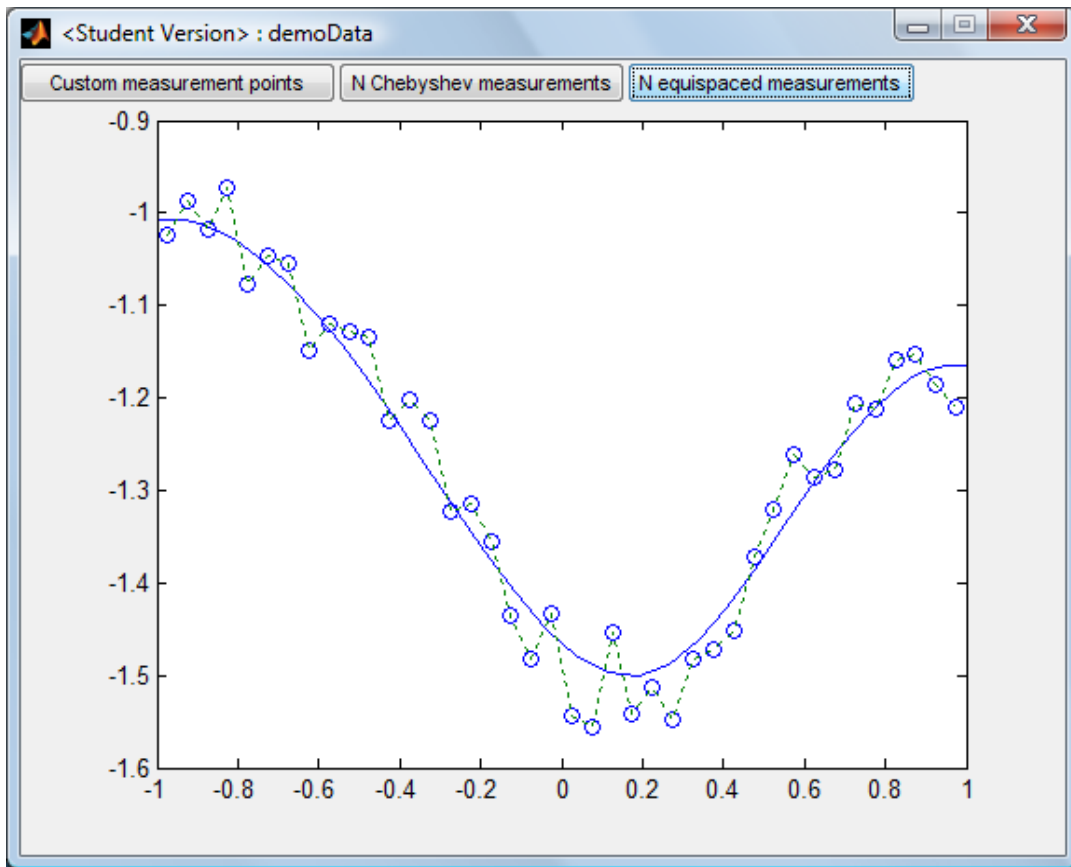


Figure 7: The true data curve and noisy data points (10% relative noise) measured on the boundary of the device.

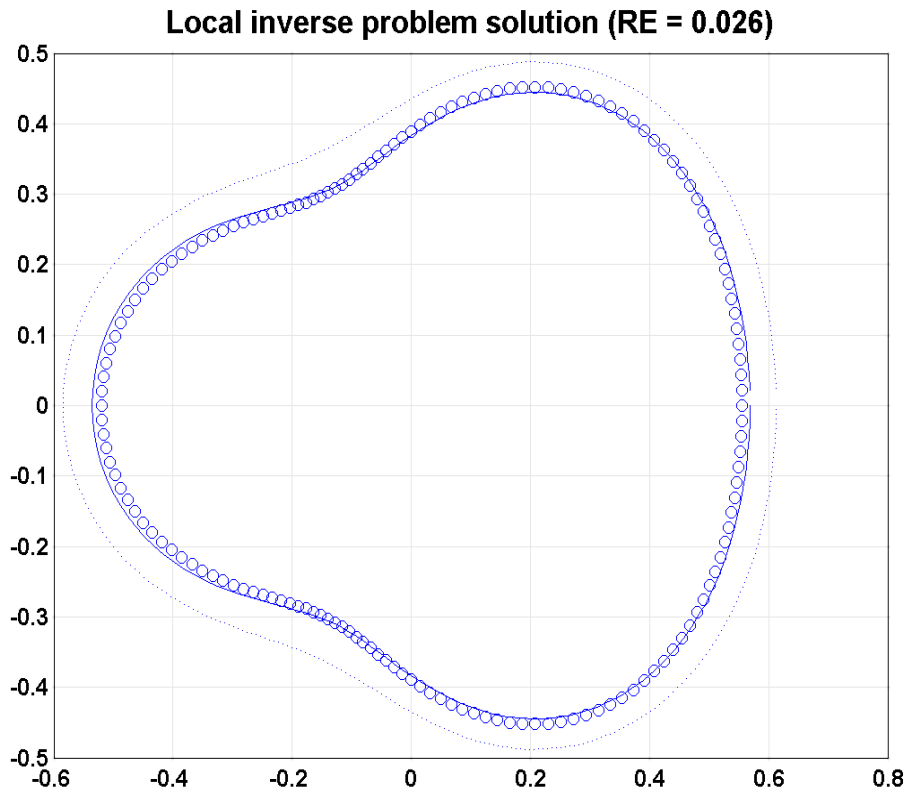


Figure 8: The solution (created only from the noisy data points and an initial guess) to the local inverse problem using Nelder-Mead simplex functional minimization search (true domain is a solid line, the reconstruction is in open circles, and the nearby initial guess—hence the term “local”, since a random, but nearby initial guess is generated—is shown in a dotted line). “RE” means relative error in the data, not in the doping profile. In cases when nonuniqueness holds, it is possible for the RE to be small, but for the reconstruction not to coincide with the original doping profile.

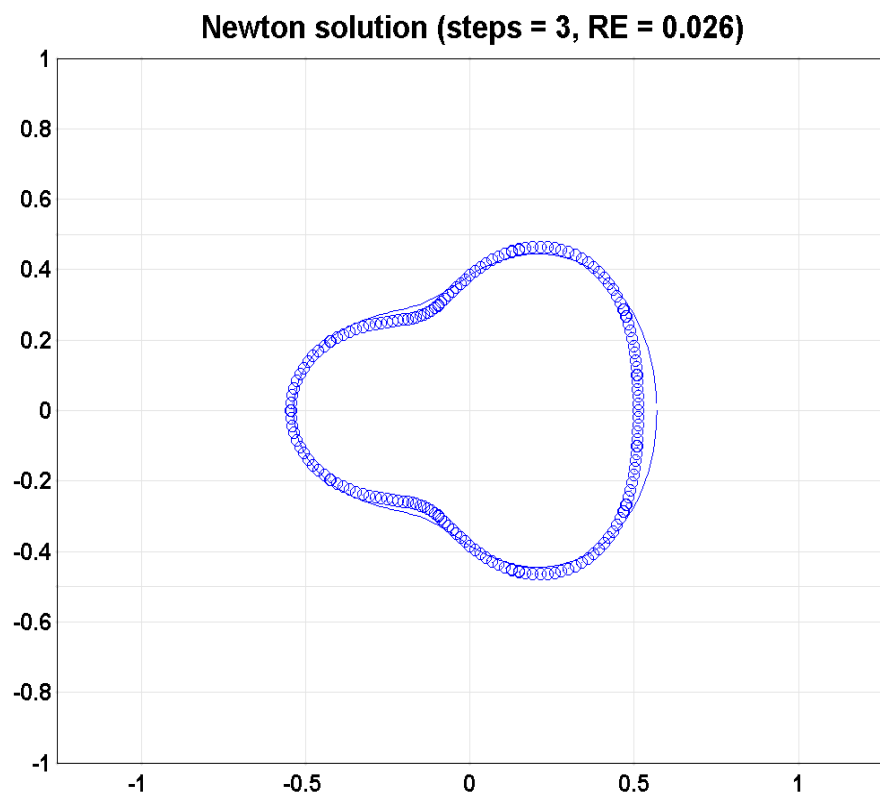


Figure 9: The solution to the local inverse problem using Newton's Method.

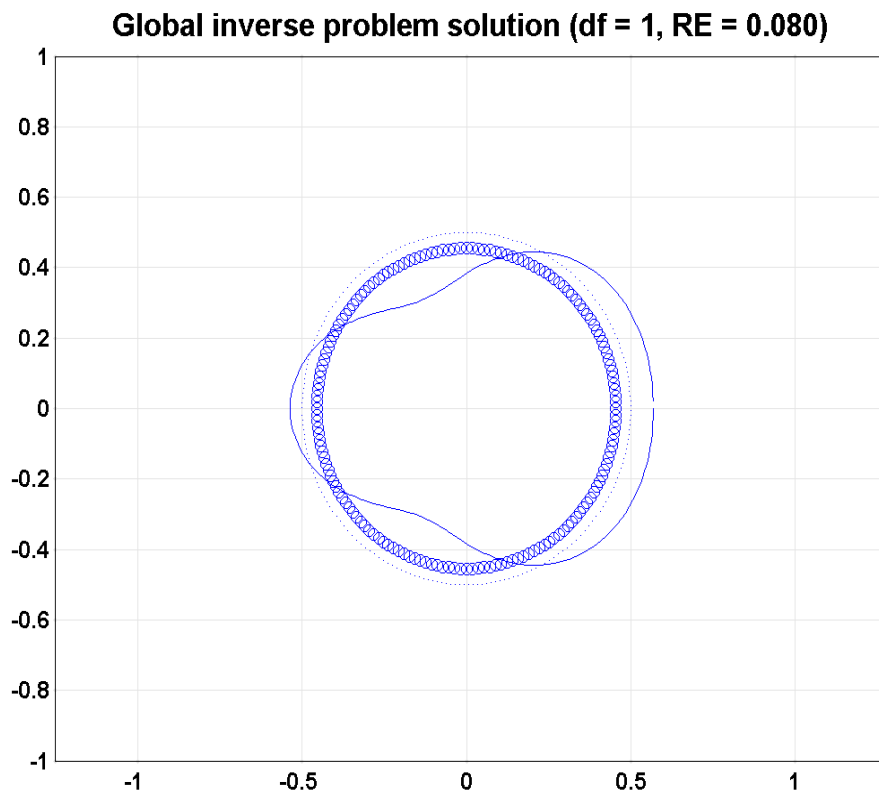


Figure 10: The solution to the global inverse problem (no prior information is known or assumed; the solution is created only from the noisy data points) with one degree of freedom.

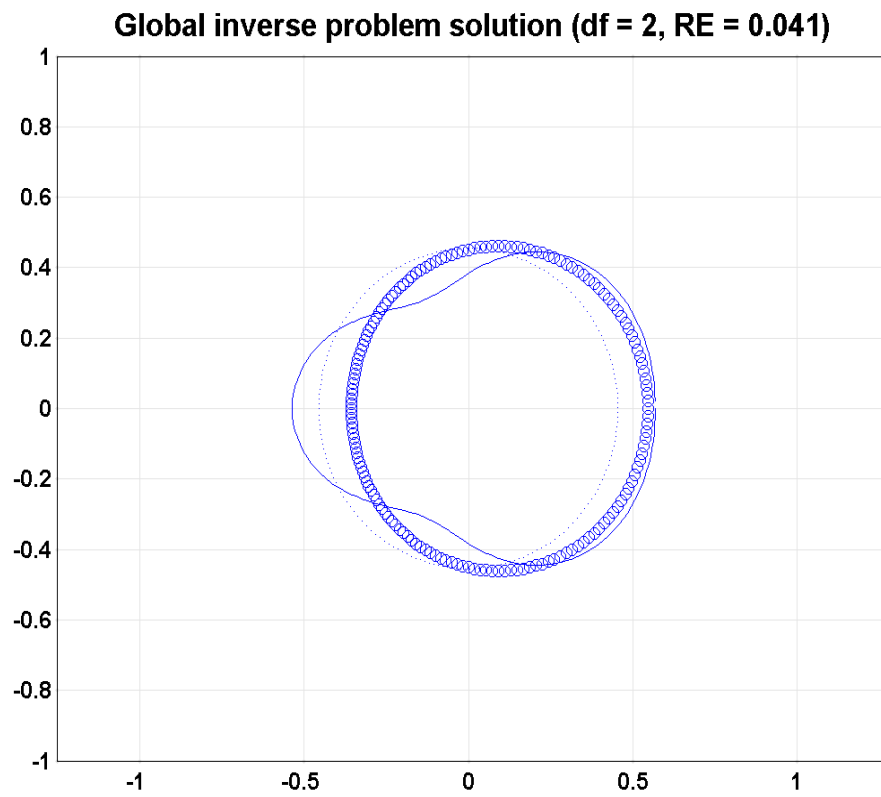


Figure 11: The solution to the global inverse problem—first with 2 degrees of freedom

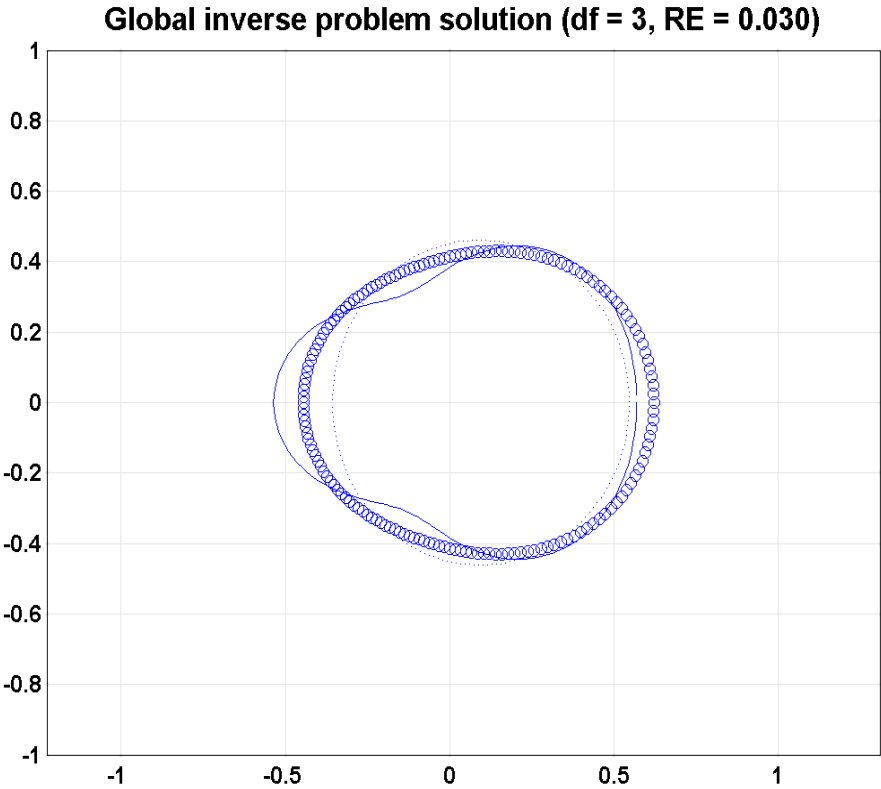


Figure 12: Then with 3 degrees of freedom

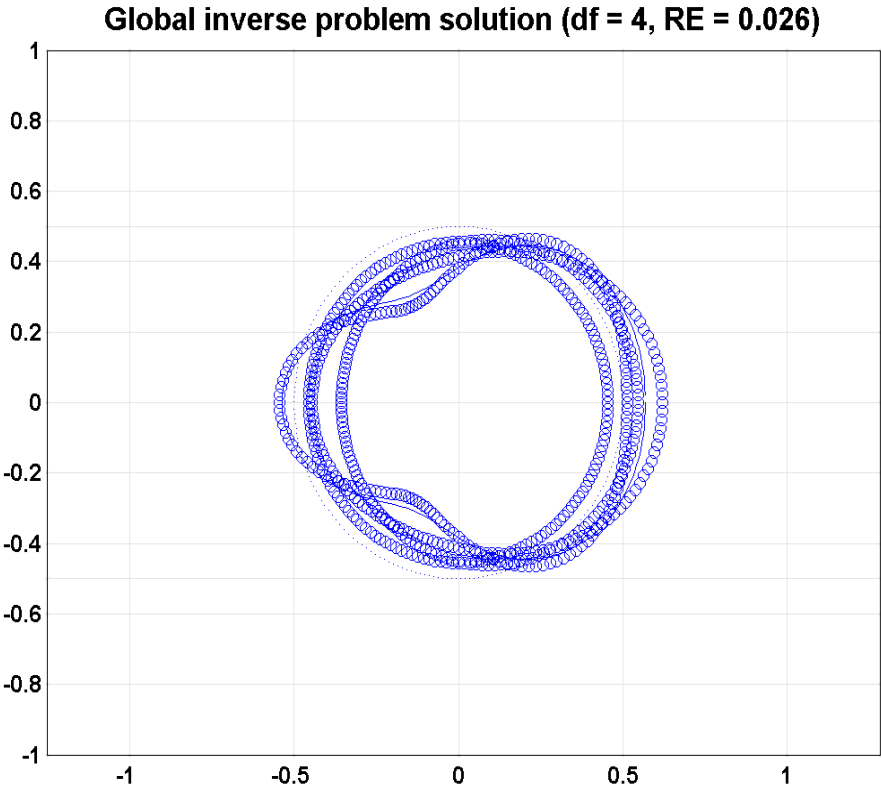


Figure 13: Lastly, with 4 degrees of freedom