

# Freeform determination of a nonlinear diffusion coefficient by a reduced adjoint system

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**Abstract.** In this article we deal with the determination of a diffusion coefficient function in a quasi-linear parabolic system. The motivation comes from a metallurgy setting. The solution method is based on the output least-squares approach (OLS) with minimization applying the adjoint equation. As the diffusion coefficient has an a-priori unknown form, we apply freeform determination in which the coefficient is defined by a linear interpolation. To avoid higher order of interpolation of the coefficient, as well as to enable the use of an adjoint system which is of the same complexity as the original partial differential equation, a reduced adjoint equation is used, applying a mapping strategy. This method is compared with a standard Levenberg-Marquardt approach.

## 1. Introduction

Diffusion processes in metallurgy are described by Fick's laws of diffusion, leading to models described by partial differential equations (PDE), see [1]. In practical applications, the material properties enter the model via the diffusion coefficient and this coefficient can depend nonlinearly on the solution of the PDE. Due to the complicated micro behaviour (phase changes, hole formation, migration), it is often more straightforward to apply a macro-diffusion coefficient hiding the underlying processes which are experimentally hard to determine.

In [2] a model and numerical discretisation suitable to the solution of the diffusion process is proposed, as well as an experimental technique usable in the determination of the unknown diffusion coefficient by an inverse method. The solution of the diffusion problem can be obtained by different techniques (e.g. finite differences [3]), however the experiment is fixed: known concentration distribution over the entire sample at discrete time steps.

The determination of unknown nonlinearities from such experiments is in general an *ill-posed* problem. Apart from the question of existence and uniqueness of the determined variables, the lack of stability implies that small measurement errors may lead to large deviation of the determined diffusion coefficient from its true value. However, the determination of the unknowns by inverse modeling in parabolic PDE is common practice, see eg [4, 5] and references therein. The ill-posedness is generally handled by introducing a generalized solution defined by the minimum of an appropriate error functional, as well as the application of regularization. Stabilization can furthermore be achieved by doing a discretization of the coefficient space, instead of considering the infinite dimensional problem.

Here we will apply the adjoint or costate method to determine the gradient of the penalty functional, see eg. [6]. The adjoint method however has the disadvantage that the resulting adjoint equation can be of a different form than the original equation, hence requiring a different solution method. We consider a pure diffusion problem, of which the common adjoint equation is a convection-diffusion problem. Furthermore, in the adjoint equation derivatives of the unknown coefficient function can appear, making a linear interpolation scheme for the determination of the coefficient function not ideal (ie. a discontinuous derivate can increase the computation time drastically).

To avoid these complications, we propose a mapping strategy, which correlates the changes of the unknown parameters to the change of the diffusion coefficient in specific space-time points. This yields the possibility of using a reduced adjoint equation consisting solely of a pure diffusion problem, and without the appearance of derivatives of the unknown diffusion coefficient.

The use of a freeform or unbiased determination of a coefficient function has been proposed in eg. [7] for a diffusion problem arising in soil sciences. The weak smoothness of a piecewise linear parametrization there leads to the use of a piecewise cubic Hermite interpolation, which will not be needed in our method. The problem of the amount of degrees of freedom and the optimal position of the interpolation points is not considered in our work. We restrict ourselves to the one dimensional case and the application of the mapping strategy; questions related to the selection of the number and position of the unknowns will be addressed in a later paper.

Application of the reduced adjoint equation has some correspondance to the technique of linearization of the original problem, as done in [4]. However, by only considering the linearization in the adjoint problem, we avoid the complications in determining the unknown nonlinear diffusion coefficient from the linearized diffusion coefficient. This means of course that a nonlinear forward problem must be solved, but this is not necessarily as problematic as it is sometimes claimed. Note that having discrete time measurements that are far apart, makes neither techniques relying on knowledge of the change over time applicable, eg. [5], nor equation error methods as in [8].

In Section 2 we give our setting: diffusion of a component in an iron bar. We also describe the experiments that are possible in order to determine the unknown diffusion coefficient, and briefly sketch the numerical discretization used to solve the forward problem. In the next section we give the standard solution of the inverse problem. In Section 4 we present our mapping strategy, and we end this article with section 5 comparing the different inverse methods based on an analytical example. We close this article with our conclusions and with ideas on how this idea can be applied to the two dimension problem arising in a ternary diffusion problem.

## 2. Nonlinear diffusion

When considering heat induced diffusion of a surface coating into a steel substrate, we only need to consider a one dimensional model. When the coating consists of several components, a multicomponent diffusion model is required. In this case, a common model reduction uses an effective binary diffusion coefficient, [1]. An  $n$ -component system is thereby reduced to a binary system by choosing one specific component,  $i$ , and a fictitious second component acting on behalf of all the other real components,  $n \neq i$ . This leads to the *nonlinear diffusion equation* for  $x \in \Omega \equiv (0, W)$  and  $t \in I \equiv (0, T)$ :

$$\partial_t c(x, t) - \partial_x (D(c(x, t)) \partial_x c(x, t)) = 0 \quad (1)$$

$$c(x, 0) = c_0(x) \quad (2)$$

$$\partial_x c(0, t) = 0 = \partial_x c(W, t), \quad (3)$$

where  $W$  is the width of the sample and  $T$  is the end time of the experiment.  $c(x, t)$  denotes the concentration of the component we are interested in, and  $c_0$  is a given smooth initial concentration. The boundary condition (3) indicates no flow boundaries.

Measurements of the sample are done as follows, [9]. The sample is cooled, effectively stopping the diffusion process. It is cut, so that the internal composition can be measured in a Scanning Electron Microscope (SEM) equipped with EDS (Energy Dispersive Spectroscopy). This gives the concentration expressed in atomic percentage, which can be converted to a standard concentration (mol/mm<sup>3</sup>).

As the measurement destroys the sample, one starts with a batch of identical samples (same initial condition), and measures at specific time steps. This translates in additional conditions,

$$c(x, t_j) = c_j(x), \quad j = 1, 2, \dots, M. \quad (4)$$

Many solution methods have been proposed for problem (1)-(3). Here we follow a *method of lines* approach. The space discretization is done by *finite volumes*, in which the interval is split in  $N$  cells, and the value of the concentration in the midpoint of the cell follows from the inflow and outflow balance, ie. the flux  $D(c)\partial_x c$  on the edges. We obtain an ODE system of  $N$  equations, which is then solved by a stiff ODE solver (we have used the Netlib lsoda implementation, [10]).

### 3. Solution of the inverse problem

#### 3.1. Set-up

The inverse problem aims at determining the diffusion coefficient  $D$ , using the information given by the measurements (4). It is clear that the domain in which  $D$  can be identified is limited by the attained values. Hence the best we can achieve is to reconstruct  $D$  over  $(c_{\min}, c_{\max})$  with  $c_{\min} = \min_{j=0, \dots, M; x \in (0, W)} c_j(x)$ , and  $c_{\max} = \max_{j=0, \dots, M; x \in (0, W)} c_j(x)$ . Due to the nature of the diffusion process, the maximum and minimum value will only be reached for a small time period, making the inverse determination at those points unstable.

The measurements (4) are discrete in time, and in practice are not continuous in space. As a consequence, consider the observations as a finite dimensional vector of observations,  $\mathbf{m} \in \mathbb{R}^n$ . Denote by  $\mathbf{m}(D)$  the observations obtained by solving the direct problem for a given diffusion coefficient  $D$ . The measurements, usually disturbed by measurement errors, are denoted by  $\mathbf{m}^*$ .

The inverse problem reads: find the diffusion coefficient  $D$ , which solves

$$\mathbf{m}(D) = \mathbf{m}^*. \quad (5)$$

A solution of (5) does not generally exist because of errors due to an inexact model or measurement deviation. Therefore, one defines a generalized solution by a least squares approach: Find  $D^*$  which minimizes

$$J(D) = \frac{1}{2} \|\mathbf{m}(D) - \mathbf{m}^*\|_2^2, \quad (6)$$

where  $\|\cdot\|_2$  denotes the Euclidian vector norm. Eq. (6) is also called the cost functional or penalty function.

When few parameters need to be determined by an inverse method, the above strategy is feasible, often leading to good results. However, in this case we want to determine a coefficient function of which no a priori information is known. Some sort of regularization will be needed in order to select the optimal generalized solution. Many techniques are possible, see eg. [11]. Here we choose to regularize by a discretization of the coefficient space, in which a finite number of parameters is used, with a minimum of correlation. If few parameters are used, no further regularization is needed, however, if many parameters are used, a total variation regularization of the diffusion coefficient makes sense in this setting. We now discuss in details the parametrisation of the coefficient function  $D$ .

### 3.2. Parametrisation of $D$

We replace the diffusion coefficient  $D(c)$  by a parametrization  $D_{\mathbf{p}}(c)$  which is continuous and piecewise analytic on  $[c_{\min}, c_{\max}]$  and is defined as follows. Let

$$c_{\min} = c_1 < c_2 < \dots < c_{r-1} < c_r = c_{\max}, \quad (7)$$

be a partition on the domain where each node  $c_j$  has an accompanying degree of freedom  $p_j$  ( $j = 1, \dots, r$ ). These values are used as values at the nodes. We set

$$D_{\mathbf{p}}(c_j) := p_j \quad \text{for } j = 1, \dots, r. \quad (8)$$

For  $c \in (c_j, c_{j+1})$ ,  $j = 1, \dots, r-1$ , the value of  $D_{\mathbf{p}}(c)$  is determined by linear interpolation between  $p_j$  and  $p_{j+1}$ , so

$$D(c) = p_j L_j(c) + p_{j+1} L_{j+1}(c), \quad \forall c \in [c_j, c_{j+1}], \quad (9)$$

with

$$\begin{cases} L_j(c) = 0, & \forall c \notin [c_{j-1}, c_{j+1}] \\ L_j(c) = \frac{c-c_{j-1}}{c_j-c_{j-1}}, & \forall c \in [c_{j-1}, c_j] \\ L_j(c) = \frac{c_{j+1}-c}{c_{j+1}-c_j}, & \forall c \in [c_j, c_{j+1}] \end{cases} \quad (10)$$

The use of linear interpolation is important here. Indeed, it guarantees that the change of one parameter  $p_j$  has a minimal influence on the coefficient function, i.e. if  $p_j$  changes, then  $D_{\mathbf{p}}(c)$  changes over  $(c_{j-1}, c_{j+1})$ . Most interpolation methods do not have this property and show a global dependance, with the advantage however that the first, or even the second derivative can be continuous. In [7] a piecewise cubic Hermite interpolation is used for a coefficient function which exhibits a local behaviour. This is feasible there as the coefficient function is monotone, allowing for an interpolation with continuous first derivative and local character, however a selection algorithm is needed to determine an optimal interpolation, which indicates a degree of freedom which is not controlled in the inverse problem.

For our non-monotone data, we could use the cubic Hermite interpolation by dividing the domain in monotonic pieces with homogeneous Neumann border conditions. A change of a parameter can have local character if the piecewise monotone structure is preserved. As we adopt a strategy that does not depend on the derivative of the diffusion coefficient, we choose the simple linear interpolation instead of the above technique.

The inverse problem then reads: Find  $\mathbf{p}^*$  which minimizes

$$J(\mathbf{p}) = \frac{1}{2} \|\mathbf{m}(D_{\mathbf{p}}) - \mathbf{m}^*\|_2^2. \quad (11)$$

This functional  $J$  is minimized by constructing an adjoint problem to calculate its gradient.

### 3.3. The adjoint problem

Use of an adjoint problem is a standard method to solve the inverse problem. In this case, we consider a continuous version of the least squares functional,

$$J(\mathbf{p}) = \frac{1}{2} \left\| \left( \sum_{j=1, \dots, M} \delta(t - t_j) \right)^{\frac{1}{2}} (c(D_{\mathbf{p}}) - c^*) \right\|_{L_2(\Omega \times I)}^2, \quad (12)$$

where  $\delta$  is the Dirac measure, and  $c^*(x, t)$  is a suitable interpolation of the measurement over the entire domain. The diffusion coefficient depends on the concentration and on the parameters,

so  $D_{\mathbf{p}} \equiv D(c, \mathbf{p})$ . The adjoint equation corresponding to (1) and (12) satisfies the end value problem:

$$\partial_t \psi(x, t) + \partial_x (D_{\mathbf{p}} \partial_x \psi(x, t)) - D'_{\mathbf{p}} \partial_x c \partial_x u = (c(x, t) - c^*) \sum_{j=1, \dots, M} \delta(t - t_j) \quad (13)$$

$$\psi(x, T) = 0 \quad (14)$$

$$\partial_x (D(c) \psi(0, t)) = 0 = \partial_x (D(c) \psi(W, t)), \quad (15)$$

with  $x \in \Omega$  and  $t \in I$  and  $D'_{\mathbf{p}} = \frac{dD(c, \mathbf{p})}{d\mathbf{p}}$ . The solutions  $c(x, t)$  and  $\psi(x, t)$  yield the gradient of (12)

$$\partial_{p_j} J(\mathbf{p}) = \int_0^T \int_0^W \partial_{p_j} D_{\mathbf{p}} \partial_x c \partial_x \psi \, dx dt. \quad (16)$$

The inverse problem is hence usually solved by the following algorithm

- (i) Choose a valid starting value  $\mathbf{p}_1$ ,  $j = 1$ .
- (ii) Obtain solution  $c_j(x, t)$  of the direct problem (1)-(3) for  $\mathbf{p}_j$
- (iii) Solve adjoint problem (13)-(15) for  $\mathbf{p}_j$  and  $c_j$ .
- (iv) Determine the gradient of the cost functional with (16).
- (v) Determine a new value  $p_{j+1}$  by application of a suitable gradient optimization method (eg. conjugate gradient method).
- (vi) Stop if stopping criterium is satisfied, otherwise:  $j = j + 1$  and go to (ii).

As stopping criterium several choices are possible. Here we opt for the easily implemented discrepancy principle, [12].

However, the above algorithm has the following problems:

- The adjoint problem (13) is of convection-diffusion type, which means that a suitable numerical method must be used.
- The derivate of the diffusion coefficient  $D'_{\mathbf{p}}$  must be well defined and must be a good approximation of the real derivative.

To avoid the above problems, we propose in the next section a different strategy.

#### 4. A mapping strategy

Let  $\phi$  be the solution of the following adjoint problem, which we will call the reduced adjoint problem:

$$\partial_t \phi(x, t) + \partial_x (D_{\mathbf{p}} \partial_x \phi(x, t)) = (c(x, t) - c^*) \sum_{j=1, \dots, M} \delta(t - t_j) \quad (17)$$

$$\phi(x, T) = 0 \quad (18)$$

$$\partial_x (D(c) \phi(0, t)) = 0 = \partial_x (D(c) \phi(W, t)). \quad (19)$$

The variation of the least squares functional (12) can be expressed as

$$\delta J(\mathbf{p}) = \int_0^T \int_0^W \delta D_{\mathbf{p}} \partial_x c \partial_x \phi \, dx dt. \quad (20)$$

Here  $\delta D_{\mathbf{p}}$  corresponds to the variation in the diffusion coefficient by a change  $\delta \mathbf{p}$  in the parameters  $\mathbf{p}$ . Discretization of the variation leads to the approximation:

$$\delta J(\mathbf{p}) = \sum_{k=0}^{K-1} \sum_{l=0}^{L-1} \delta D_{\mathbf{p}}(x_{k+\frac{1}{2}}, t_l) \partial_x c(x_{k+\frac{1}{2}}, t_l) \partial_x \phi(x_{k+\frac{1}{2}}, t_l) \Delta_k \Delta t, \quad (21)$$

where we have used the following partitions: let  $\{x_k\}_{k=0}^K$  be a partition of  $\Omega$ ,  $\Delta_k = x_{k+1} - x_k > 0$ ,  $x_0 = 0$ ,  $x_K = W$ ,  $x_{k+\frac{1}{2}} = \frac{x_k + x_{k+1}}{2}$ , and  $\{t_l\}_{l=0}^L$  a partition of  $I$  with  $t_l = l\Delta t$ ,  $\Delta t = T/L$

In order to calculate (4) we need to determine the variation in the diffusion coefficient on specific space and time points. We have that

$$\begin{aligned} \delta D_{\mathbf{p}}(x_{k+\frac{1}{2}}, t_l) &= \delta D(c(x_{k+\frac{1}{2}}, t_l), \mathbf{p}) \\ &= \delta p_j L_j(c(x_{k+\frac{1}{2}}, t_l)) + \delta p_{j+1} L_{j+1}(c(x_{k+\frac{1}{2}}, t_l)) \quad \text{with } c(x_{k+\frac{1}{2}}, t_l) \in [c_j, c_{j+1}] \\ &= \sum_j m_{jk}^l \delta p_j = \left( \delta \mathbf{p}^T \mathbf{M}^l \right)_k, \end{aligned}$$

here the mapping matrix  $M^l \in \mathbb{R}^{r \times K}$  for every time step  $t_l$  is a sparse matrix with two non-zero elements in every column. This matrix allows us to determine  $\delta D_{\mathbf{p}}$ . The superscript  $T$  indicates the transpose operation.

To approximate the derivative in space of a function in the midpoints by the values of the function in the midpoints themselves introduce the notation,  $\mathbf{L} \in \mathbb{R}^{K \times K}$ :

$$\mathbf{L} = \begin{pmatrix} \frac{-1}{\Delta_{\frac{1}{2}}} & \frac{1}{\Delta_{\frac{1}{2}}} & & & \\ \frac{-1}{\Delta_{\frac{1}{2}} + \Delta_{\frac{3}{2}}} & 0 & \frac{1}{\Delta_{\frac{1}{2}} + \Delta_{\frac{3}{2}}} & & \\ & \ddots & \ddots & & \\ & & \frac{-1}{\Delta_{K-\frac{5}{2}} + \Delta_{K-\frac{3}{2}}} & 0 & \frac{1}{\Delta_{K-\frac{5}{2}} + \Delta_{K-\frac{3}{2}}} \\ & & & \frac{-1}{\Delta_{K-\frac{3}{2}}} & \frac{1}{\Delta_{K-\frac{3}{2}}} \end{pmatrix}, \quad (22)$$

with  $\Delta_{k+\frac{1}{2}} = \frac{1}{2}(\Delta_k + \Delta_{k+1})$ . The remaining terms in ( ) can now be calculated. We have that  $\partial_x c(x_{k+\frac{1}{2}}) = (\mathbf{L} \mathbf{c})_k$ , where  $\mathbf{c}$  is the vector with elements  $c(x_{k+\frac{1}{2}})$ , and the same for  $\phi$ , so  $\partial_x \phi(x_{k+\frac{1}{2}}) = (\mathbf{L} \mathbf{f})_k$ , where  $\mathbf{f}$  is the vector with elements  $\phi(x_{k+\frac{1}{2}})$ . If we next introduce the vector  $\mathbf{g}^l$  with elements  $g_i = (\mathbf{L} \mathbf{c})_i (\mathbf{L} \mathbf{f})_i \Delta_i \Delta t$  taken at  $t = t_l$ , we obtain for the variation of the functional

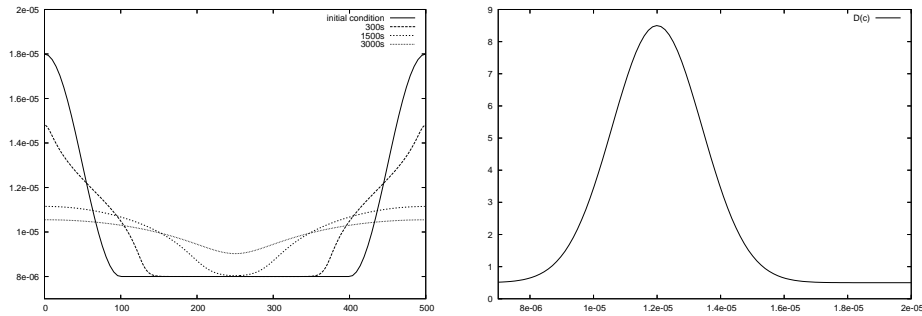
$$\delta J(\mathbf{p}) = \sum_{l=0}^{L-1} \sum_{k=0}^{K-1} \left( \delta \mathbf{p}^T \mathbf{M}^l \right)_k \mathbf{g}_k^l = \sum_{l=0}^{L-1} \delta \mathbf{p}^T \mathbf{M}^l \mathbf{g}^l. \quad (23)$$

It follows that the gradient of the functional can be calculated by

$$\partial_{p_j} J(\mathbf{p}) = \sum_{l=0}^{L-1} (\mathbf{M}^l \mathbf{g}^l)_j. \quad (24)$$

The inverse algorithm is then

- (i) Choose a valid starting value  $\mathbf{p}_1$ ,  $j = 1$ .
- (ii) Obtain solution  $c_j(x, t)$  of the direct problem (1)-(3) for  $\mathbf{p}_j$
- (iii) Solve adjoint problem (17)-(19) for  $\mathbf{p}_j$  and  $c_j$ .
- (iv) Calculate  $\mathbf{M}^l$  and  $\mathbf{g}^l$
- (v) Determine the gradient of the cost functional with (24).
- (vi) Determine a new value  $p_{j+1}$  by application of a suitable gradient optimization method (eg. conjugate gradient method).
- (vii) Stop if stopping criterium is satisfied, otherwise:  $j = j + 1$  and go to (ii).



**Figure 1.** Concentration profiles at  $t = 0, 300, 1500$  and  $3000$  seconds, and the diffusion profile  $D(c)$  that generates these.

As the adjoint equation (17) is of the same form of the direct problem (but now a linear variable coefficient diffusion problem), the same solution method can be used as for the direct problem. The reaction term on the right hand side must be treated carefully due to the appearance of a Dirac measure. One has to solve the problem over the interval  $(t_j, t_{j+1})$ , starting from  $t_{j+1}$  without reaction, from which one obtains the value  $\bar{\phi}(x, t_j)$ . Next one has to apply the reaction as

$$\phi(x, t_j) = \bar{\phi}(x, t_j) + (c(x, t_j) - c^*).$$

This is then the end condition for the next time slice  $(t_{j-1}, t_j)$ .

### 5. Numerical Example

In Section 3 we have presented the standard adjoint method for the nonlinear diffusion problem, and in Section 4 the reduced adjoint method. In the following numerical example we will compare the results of a steepest descent search using the calculated gradient, with the results obtained by the Levenberg-Marquardt problem, see [13], which is a trust region method based on finite difference determination of the gradient by means of many solutions of the direct problem. Netlib, [10], contains a reference implementation in Fortran that can be used.

We take the following initial condition,  $x \in (0, 500)$ :

$$c_0(x) = \begin{cases} 0.5 \cdot 10^{-5} (1 + \cos(\frac{\pi x}{100})) + 8 \cdot 10^{-6}, & x \leq 100 \\ 8 \cdot 10^{-6}, & 100 < x < 400 \\ 0.5 \cdot 10^{-5} (1 + \cos(-\frac{\pi(x-500)}{100})) + 8 \cdot 10^{-6}, & x \geq 400. \end{cases}$$

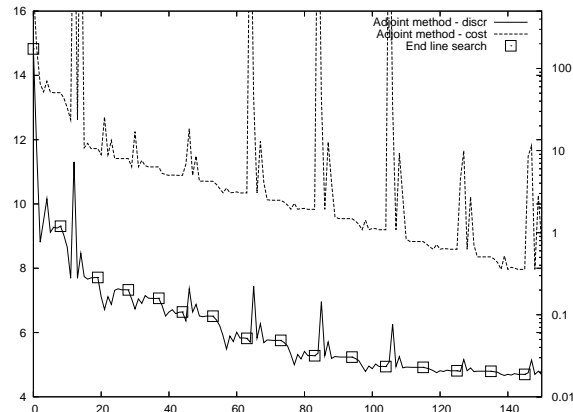
We solve the direct problem for a diffusion coefficient given by

$$D(c) = 8 \exp \left( - \left( \frac{10^5 c - 1.2}{0.2} \right)^2 \right) + 0.5,$$

and consider the solution at  $t = 300, 1500$  and  $3000$  seconds as the experimental values  $c^*$ , see Fig. 1. This example resembles the experimental setup, albeit with reduced times (experimental times can be up to 3 hours) to limit the computational time (especially for Levenberg-Marquardt that needs many solution of the direct nonlinear problem).

For the inverse problem, we consider the following partition of the concentration interval:

$$10^{-5} \{0.79, 0.85, 0.9, 0.95, 1, 1.15, 1.2, 1.25, 1.3, 1.35, 1.4, 1.45, 1.5, 1.55, 1.6, 1.7, 1.85\},$$



**Figure 2.** Results of the reduced adjoint method. The  $x$ -axis denotes the number of solutions of the direct problem. The boxes denote the 16 iterations where the gradient was calculated, the top curve is the cost functional expressed in log scale, and the lower curve the discrepancy.

where we have taken the minimum and maximum value outside of the interval  $[c_{\min}, c_{\max}]$ , ie.  $0.79 \cdot 10^{-5} < 0.8 \cdot 10^{-5} = c_{\min}$ . To deal with stability problems we have taken larger steps towards  $c_{\max}$ . We have also taken a big step after  $c = 10^{-5}$  in order to break the equidistant steps. The partition has 17 nodes, hence there will be 17 unknown parameters in the inverse problem, that is,  $\mathbf{p} \in \mathbb{R}^{17}$ . As starting value for the inverse algorithm we take  $p_i = 1$ .

To measure the performance of the different methods, we calculate the discrepancy between the retrieved parameters  $\mathbf{p}^*$ , and the exact values  $D(c_i)$ . This discrepancy is the vector norm of the distance between these two vectors.

In Fig. 2 the results as obtained by the reduced adjoint method are shown. The  $x$ -axis denotes the number of solutions of the direct problem. In this, 16 evaluations of the adjoint system were needed, the rest of the time was spent doing a line search in the gradient direction. The top curve is the value of the cost functional, which is used in the determination of the diffusion coefficient. The peaks are a consequence of the line search that overshoots the minimum. The bottom line shows the discrepancy. As is common in this type of method, the line search takes a large amount of the computational time. The result however clearly validates the approach of using the reduced adjoint equation to calculate the gradient.

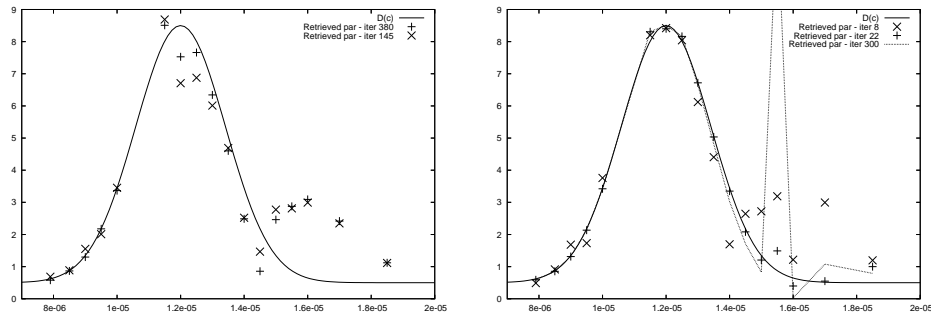
The resulting diffusion coefficient is depicted in Fig. 3 (Left). The result after 145 and 380 direct evaluations are given. For 145 iterations, this corresponds to 15 evaluations of the adjoint problem. Good identification is retrieved for the lower concentration values, with the discrepancy getting larger towards the maximum concentration values.

Next we recover the diffusion coefficient applying the Levenberg-Marquardt method. To avoid problems with negative diffusion values, we optimize for parameters  $q_i$  defined as  $q_i = \ln(p_i)$ . The resulting cost and discrepancy are given in Fig. 4. The left figure gives the first 22 cost functional evaluations. As there are 5 bad evaluation, this means there have been 17 gradient evaluations, or a total of 294 evaluations of the direct problem. The right of Fig. 4 shows the typical long time behaviour of inverse methods if no stopping criterium is used: improvement of cost while the discrepancy increases again.

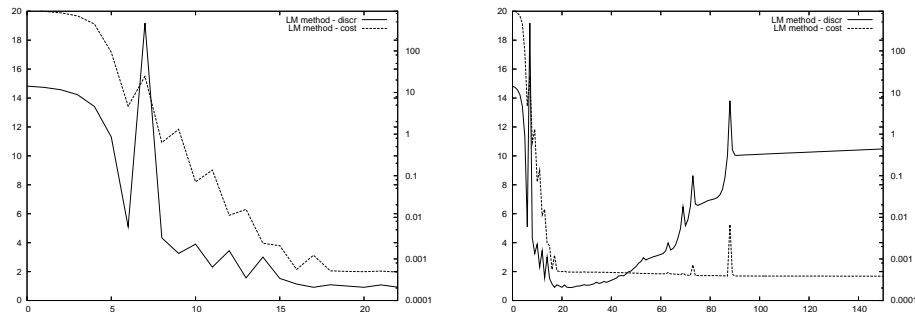
The right of Fig. 3 shows the retrieved diffusion coefficient for the LM method.

Comparing the two methods, we need to compare the LM on iteration 8 to the reduced adjoint method on iteration 145, which corresponds to equal computational effort. Both give comparable results.





**Figure 3.** Retrieved diffusion coefficient. Left with Adjoint method, right with Levenberg-Marquardt.



**Figure 4.** Results of the Levenberg-Marquardt method. The  $x$ -axis denotes the number of cost functional evaluations, where each reduced cost, leads to an extra 17 evaluations of the direct problem (gradient determination). The top curve is the cost functional expressed in log scale, and the lower curve the discrepancy.

## 6. Conclusion

We have explained how a reduced adjoint method can be used in a diffusion coefficient optimization process. The obtained results are comparable to existing methods like the Levenberg-Marquardt method. The advantage of the method is that it has all benefits of an adjoint method (no penalty on number of parameters, that is, usable for higher dimensional diffusion coefficients), while still avoiding some of the drawbacks of applying the full adjoint equation: different PDE than the direct equation, regularity of the diffusion coefficient needed.

Having shown the feasibility of the method, we plan to apply it to metallurgy experiments with ternary alloys, where the diffusion coefficient is a two-dimensional surface.

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