3-D shape and contrast reconstruction in optical tomography with level sets

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Abstract. Many applications of optical tomography in medical diagnostics, including the imaging of haematoma and tumours or the localisation of organs marked by a contrast agent, require the detection and localisation of well-defined boundaries between a homogeneous or weakly varying background and inclusions of different optical parameters. Shape-based reconstruction techniques, such as level sets, are better suited to solve these problems than conventional voxel-based approaches, which often lead to blurring of the boundaries of features and loss of contrast. In this paper we present a level set technique for the simultaneous recovery of absorption and diffusion distributions in a three-dimensional scattering medium. Images reconstructed from simulated frequency-domain boundary measurements are compared to a voxel-based conjugate gradient method. The results demonstrate the feasibility of the level set method.

1. Introduction
Optical diffusion tomography (ODT) is an imaging technique that recovers the optical parameters of a heterogeneous scattering medium from boundary measurements of light transmission. The main applications are in medical imaging, where the reconstructed absorption and scattering volume parameter distributions can be related to physiological states and processes such as oxygenation levels, oxygen uptake and metabolism rates. The proposed uses include the monitoring of oxygenation levels in term and preterm infants, brain activation studies, and breast tumour screening.

Image reconstruction methods are generally formulated as a model-based optimisation problem, where a model of light transport in scattering media is compared to the measurement data, and the parameters of the model are iteratively updated such as to minimise the difference to the measured data. The most common light transport models in ODT are the radiative transfer equation \[1, 2, 3, 4\], and, in highly-scattering problems, the diffusion approximation \[5, 6, 7\]. Given a domain \(\Omega\) bounded by \(\partial\Omega\) the diffusion equation in the frequency domain is given by

\[\begin{align*}
-\nabla \cdot \kappa(x) \nabla \Phi(x; \omega) + \left(\mu(x) + \frac{i\omega}{c}\right) \Phi(x; \omega) &= 0 \quad x \in \Omega \setminus \partial\Omega \quad (1) \\
\Phi(m; \omega) + 2\zeta \kappa(m) \frac{\partial\Phi(m; \omega)}{\partial\nu} &= f(m; \omega) \quad m \in \partial\Omega \quad (2)
\end{align*}\]
where $\mu$ and $\kappa$ are the absorption and diffusion coefficients, $\omega$ is the source modulation frequency, $\Phi$ is the photon density, $\zeta$ is a term incorporating refractive index mismatches along $\partial \Omega$ [8, 9], $\nu$ is the outward normal of the boundary at a point $m$, and $f$ is a boundary source distribution. The measurable exitance is given by the outgoing radiation

$$y(m; \omega) = -\kappa(m) \frac{\partial \Phi(m; \omega)}{\partial \nu}, \quad m \in \partial \Omega. \quad (3)$$

The forward model defined by Eqns. 1-3 can be formally described as an operator $A$ mapping from parameter to data space:

$$G = A(\kappa, \mu). \quad (4)$$

In general, Eq. 4 must be solved numerically. In this paper we use a finite element model that subdivides $\Omega$ into non-overlapping elements of simple shapes, joined at vertex nodes. Parameter distributions over $\Omega$ are then approximated by a piecewise polygonal basis expansion with limited support. This transforms (4) into a finite-dimensional linear system of equations which can be solved with standard direct or iterative methods.

Traditionally, the inverse problem of recovering the coefficients of parameter distribution $(\kappa, \mu)$ is approached by an iterative method of recovering parameter values of individual voxels or nodes, using either the same basis expansion as the forward model, or mapping into a separate basis. Common choices for the inverse solver are methods that use either first order derivative information (such as nonlinear conjugate gradients) [10] or second order derivative information (such as Newton-type methods) [11, 12, 7, 13]. Generally regularisation is required to suppress artefacts.

In more details, given some measured data $\tilde{G}$, we can define for each given pair $(\kappa, \mu)$ the data misfit described by the residual operator

$$R(\kappa, \mu) = A(\kappa, \mu) - \tilde{G}.$$ 

The typical approach for solving this inverse problem is to formulate a least squares cost functional

$$J(\kappa, \mu) = \frac{1}{2} ||R(\kappa, \mu)||^2, \quad (5)$$

possibly augmented by some additional regularisation terms, and to minimise this least squares data misfit by an iterative technique.

In many biomedical applications, the parameter distribution which is sought in the inverse problem, contains some sorts of interfaces. These can for example be boundaries of some tumour or haematoma, or the interfaces between different organs or tissue types, or the boundaries of regions filled with some tracer or marker substance. These interfaces are typically not recovered well in classical reconstruction schemes due to the above mentioned need for relatively strong regularisation tools. Most of these regularisation tools penalise variations or gradients in the parameter distribution, which yields over-smoothed reconstructions. Therefore, interfaces and boundaries are blurred and region boundaries cannot easily be detected. However, in many applications it is important to be able to find the boundaries of certain inclusions as accurately as possible. Whereas inside and outside these sub-regions the parameters might not vary much, often across the interfaces significant jumps occur in the tissue parameters. The level set technique proposed in this paper aims at providing a tool which is able to reconstruct interfaces in the region of interest together with certain characteristics of the interior and exterior sub-regions. In this paper we will concentrate on the easiest case where interior and exterior profiles are assumed to be approximately constant where these constants might either be known a priori or they might be part of the inverse problem as well. We mention that our approach can easily be generalised to more complex scenarios such as smoothly varying or parametrised interior and
exterior parameter profiles, and we plan to investigate such situations in our future work. We mention also that we have previously applied a similar method to 2D problems [14]. In the current work we extend the level set approach to 3-D problems.

2. Methods
Let us introduce two (smoothly varying) real-valued level set functions $\varphi$ and $\psi$ defined on $\Omega$. Furthermore let us assume that the unknown parameter profile in the domain $\Omega$ can be described by

$$
\kappa(x) = \begin{cases} 
\kappa_{\text{obj}} & \text{where } \varphi \leq 0, \\
\kappa_{bg} & \text{where } \varphi > 0,
\end{cases}
$$

(6)

$$
\mu(x) = \begin{cases} 
\mu_{\text{obj}} & \text{where } \psi \leq 0, \\
\mu_{bg} & \text{where } \psi > 0.
\end{cases}
$$

(7)

We assume that the background absorption and diffusion parameters $\mu_{bg}$ and $\kappa_{bg}$ are constant and known. The unknowns of the inverse problem are therefore the interior absorption and diffusion parameters $\mu_{obj}$ and $\kappa_{obj}$ (which are as well assumed to be constant) and the two level set functions $\varphi$ and $\psi$ defining the interfaces. We formulate the output least squares cost functional

$$
\mathcal{J} (\kappa(\varphi, \kappa_{obj}), \mu(\psi, \mu_{obj})) = \frac{1}{2} \| \mathcal{R} (\kappa(\varphi, \kappa_{obj}), \mu(\psi, \mu_{obj})) \|^2. 
$$

(8)

The goal is to find a minimiser $(\varphi, \psi, \kappa_{obj}, \mu_{obj})$ of this cost functional.

Notice that in classical approaches two (typically smoothly varying) functions $\kappa$ and $\mu$ need to be reconstructed from the boundary data, whereas in our new formulation two level set functions $\varphi$ and $\psi$ and two constant parameters $\mu_{obj}$ and $\kappa_{obj}$ need to be determined. We mention that, in the general case, $\mu_{obj}$, $\mu_{bg}$ and $\kappa_{obj}$, $\kappa_{bg}$ might be considered unknown smoothly varying functions as well such that the complexity of the inverse problem increases to the recovery of six unknown functions instead of two in the classical approach. We will not consider this case here, but mention that the increased complexity can be dealt with by introducing sufficient regularisation for the parameter functions in each individual sub-region as well as for the two level set functions describing the boundaries of the sub-regions.

For solving the inverse problem we adopt an evolution approach. In this approach, the unknowns of the inverse problem are assumed to depend on an artificial evolution time $t$ and evolve during the reconstruction according to the evolution laws

$$
\frac{d \varphi}{dt} = f(t), \\
\frac{d \psi}{dt} = g(t), \\
\frac{d \mu_{obj}}{dt} = h_\mu(t), \\
\frac{d \kappa_{obj}}{dt} = h_\kappa(t).
$$

(9)

(10)

The goal is to find forcing terms $f, g, h_\mu$ and $h_\kappa$ which point into a descent direction of the cost (8). For finding such descent directions, we write (6), (7) in a slightly different form

$$
\kappa = (\varphi) + \kappa_{obj} (1 - H(\varphi)),
$$

(11)

$$
\mu = (\psi) + \mu_{obj} (1 - H(\psi)),
$$

(12)

where $H$ denotes the Heaviside function. With the parameters also the cost depends on the evolution time: $\mathcal{J} = \mathcal{J}(t)$. Formal differentiation with respect to evolution time yields by the chain rule

$$
\frac{d \mathcal{J}}{dt} = \frac{\partial \mathcal{J}}{\partial \kappa} \left[ \frac{\partial \kappa}{\partial \varphi} \frac{d \varphi}{dt} + \frac{\partial \kappa}{\partial \kappa_{obj}} \frac{d \kappa_{obj}}{dt} \right] + \frac{\partial \mathcal{J}}{\partial \mu} \left[ \frac{\partial \mu}{\partial \psi} \frac{d \psi}{dt} + \frac{\partial \mu}{\partial \mu_{obj}} \frac{d \mu_{obj}}{dt} \right].
$$

(13)
Let $\mathcal{R}'_{\kappa,\mu}$ and $\mathcal{R}'_{\mu,\kappa}$ be the Fréchet derivatives of the residual operator $\mathcal{R}(\kappa,\mu)$ with respect to $\kappa$ and $\mu$ in the point $(\kappa,\mu)$ and let $\mathcal{R}'_{\kappa,\mu}^*$ and $\mathcal{R}'_{\mu,\kappa}^*$ be their adjoint operators. We will denote for brevity
\[
\operatorname{grad}_{\kappa}[\kappa,\mu] = \mathcal{R}'_{\kappa,\mu}^* \mathcal{R}(\kappa,\mu), \quad \operatorname{grad}_{\mu}[\kappa,\mu] = \mathcal{R}'_{\mu,\kappa}^* \mathcal{R}(\kappa,\mu).
\]
Then we can write (13) as
\[
\frac{d\mathcal{J}}{dt} = \Re \left\langle \operatorname{grad}_{\kappa}[\kappa,\mu], \frac{\partial\kappa}{\partial\varphi} f(t) \right\rangle + \Re \left\langle \operatorname{grad}_{\kappa}[\kappa,\mu], \frac{\partial\kappa}{\partial\psi} \right\rangle \mathcal{H}_n(t) + \Re \left\langle \operatorname{grad}_{\mu}[\kappa,\mu], \frac{\partial\mu}{\partial\varphi} g(t) \right\rangle + \Re \left\langle \operatorname{grad}_{\mu}[\kappa,\mu], \frac{\partial\mu}{\partial\psi} \right\rangle \mathcal{H}_\mu(t). \tag{14}
\]
Notice that $\mathcal{H}_n(t)$ and $\mathcal{H}_\mu(t)$ do not depend on the space variable $x$ (since the interior parameters of the inclusion are assumed constant) but that $f(t)$ and $g(t)$ do depend on it (even though this dependence has been suppressed in the notation). This has been taken into account in the above equation. Formally we get from (11), (12)
\[
\frac{\partial\kappa}{\partial\varphi} = (\kappa_{bg} - \kappa_{obj}) \delta(\varphi), \quad \frac{\partial\kappa}{\partial\psi} = 1 - H(\varphi),
\]
\[
\frac{\partial\mu}{\partial\varphi} = (\mu_{bg} - \mu_{obj}) \delta(\psi), \quad \frac{\partial\mu}{\partial\psi} = 1 - H(\psi).
\]
Expanding the above inner products we arrive at the descent directions
\[
\dot{f}(t) = -C_\varphi(t) \Re \left\langle \operatorname{grad}_{\kappa}[\kappa,\mu](t)(\kappa_{bg} - \kappa_{obj}) \right\rangle, \tag{15}
\]
\[
\dot{\mathcal{H}}_n(t) = -C_n(t) \Re \int_\Omega \operatorname{grad}_{\kappa}[\kappa,\mu](t)(1 - H(\varphi)) \, dx, \tag{16}
\]
\[
\dot{g}(t) = -C_\psi(t) \Re \left\langle \operatorname{grad}_{\mu}[\kappa,\mu](t)(\mu_{bg} - \mu_{obj}) \right\rangle, \tag{17}
\]
\[
\dot{\mathcal{H}}_\mu(t) = -C_\mu(t) \Re \int_\Omega \operatorname{grad}_{\mu}[\kappa,\mu](t)(1 - H(\psi)) \, dx, \tag{18}
\]
where $C_\varphi(t), C_n(t), C_\psi(t)$ and $C_\mu(t)$ are positive constants which steer the velocities of each component individually. They can be chosen zero as well, in which case the corresponding quantity does not evolve in the given time step.

In the case of very noisy data we will apply some additional regularisation operator to the forcing terms $\dot{f}(t)$ and $\dot{g}(t)$ which have the effect of smoothing the boundaries of the shapes during the evolution by projecting the updates towards a smoother subspace [15]. These smoothed forms of our descent directions are given as
\[
\hat{f}(t) = (\alpha I - \beta \Delta)^{-1} \dot{f}(t), \quad \hat{g}(t) = (\alpha I - \beta \Delta)^{-1} \dot{g}(t),
\]
where $\Delta$ denotes the Laplace operator and $\alpha > 0$ and $\beta > 0$ are suitably chosen regularisation parameters (good choices are, e.g., $\alpha = 1$ and $\beta = 0.08$). These will be the flows which we use in our numerical experiments.

Discretising (9), (10) by a straightforward finite difference time-discretisation with time-step $\tau > 0$ and interpreting $\varphi^n = \varphi(n\tau)$, $n = 0, 1, 2, \ldots$, (and similarly for the other evolving quantities), we arrive at the iterations
\[
\varphi^{(n+1)} = \varphi^{(n)} + \tau \hat{f}^{(n)}, \quad \psi^{(n+1)} = \psi^{(n)} + \tau \hat{g}^{(n)}, \tag{19}
\]
\[
\kappa_{obj}^{(n+1)} = \kappa_{obj}^{(n)} + \tau \hat{r}_\kappa^{(n)}, \quad \mu_{obj}^{(n+1)} = \mu_{obj}^{(n)} + \tau \hat{r}_\mu^{(n)}. \tag{20}
\]
3. Results

This section shows the results of 3-D level set reconstructions of absorption and scattering obtained from numerically simulated light transmission data.

3.1. Cube with embedded objects

A cubic domain of size $40 \times 40 \times 40$ mm was defined with mean background optical parameters of absorption $\mu_{bg} = 0.01 \text{ mm}^{-1}$, diffusion $\kappa_{bg} = 0.33 \text{ mm}$ and refractive index $n = 1.4$. The background parameter distributions were contaminated with 5% Gaussian-distributed random noise. Into the background medium were inserted three spherical inclusions: (a) radius 5 mm, $\mu = \mu_{obj} = 0.02 \text{ mm}^{-1}$, $\kappa = \kappa_{bg} = 0.33 \text{ mm}$, (b) radius 5 mm, $\mu = \mu_{bg} = 0.01 \text{ mm}^{-1}$, $\kappa = \kappa_{obj} = 0.165 \text{ mm}$, and (c) radius 3.5 mm, $\mu = \mu_{obj} = 0.02 \text{ mm}^{-1}$, $\kappa = \kappa_{obj} = 0.165 \text{ mm}$. The locations of the inclusions are shown in Fig. 1. Cross sections through the target objects in central plane $z = 0$ are shown in the left column of Fig. 2.

The object was subdivided into a finite element mesh consisting of 4096 8-noded voxel elements and 4913 nodes. 9 sources and 16 detectors were placed on each of the 6 faces of the cube, as indicated for a single face in the image. Using the FEM diffusion model, simulated transillumination measurements of complex logarithmic exitance for a source modulation frequency of 100 MHz were then generated for all source-detector combinations, leading to a total of 5184 complex-valued boundary data. 0.5% Gaussian-distributed random noise was added to the data.

Figure 1. Locations of absorption inclusions (left) and diffusion inclusions (right) in the central $z = 0$ plane of the scattering object. The source (*) and detector locations (o) for a single surface are indicated.
Two level set reconstructions were performed for this data set: (a) shape reconstruction only, and (b) combined shape and contrast recovery. In case (a), the contrast of the inclusions was assumed to be known. In case (b), the initial contrast of the interior regions was set to $\mu^{(0)}_{obj} = 0.015 \text{mm}^{-1}$ and $\kappa^{(0)}_{obj} = 0.22 \text{mm}$, and the contrast recovery was included in the reconstruction process. The reconstruction basis was defined as a regular tri-linear voxel grid of dimension $30 \times 30 \times 30$.

For both level set reconstructions, the initial parameter distribution was set to the mean background level throughout the domain. At each iteration $k$ of the level set algorithm, an inexact line search along the calculated update direction ($\text{grad} \mu$, $\text{grad} \kappa$) was performed, such that after updating the level set functions, a target number $p^{(k)}$ of voxels was flipped from exterior to interior region or vice versa. $p^{(k)}$ was evaluated as

$$p^{(k)} = \alpha D \frac{J^{(k)}}{J^{(0)}}$$

(21)

where $D$ was the total number of voxels, and $\alpha = 0.02$ was a fixed scaling parameter.

To provide a reference, a reconstruction of the same data was performed with a conventional voxel-based reconstruction using a nonlinear conjugate gradient (CG) method with first-order Tikhonov regularisation. The reconstruction basis in this case was again a regular $30 \times 30 \times 30$ voxel grid.

Cross sections through the central plane $z = 0$ of the reconstructed images for both level set reconstructions and the CG reconstruction are shown in Fig. 2. It can be seen that the object locations and sizes are well recovered with both level set reconstructions, with small distortions to the object shapes. The combined shape and contrast reconstruction produces a small cross-talk artefact in the absorption image. By comparison, the CG reconstruction has low contrast, and the inclusions are not well defined, in particular in the absorption image. There is also some cross-talk evident in both the absorption and diffusion images.

For a quantitative comparison between the level set reconstructions and voxel-based CG reconstruction, profiles through the reconstructed images are shown in Fig. 3. The profiles are
Figure 3. Profiles of the reconstructed absorption (left) and diffusion images (right) through the inclusions, for both level set reconstructions and the CG reconstruction.

Figure 4. Contrast evolution during combined shape and contrast reconstruction for absorption and scattering images, as a function of iteration index. Target values are shown as dashed lines.

displayed along the line $x = 10, z = 0$ for $\mu$, and $y = -10, z = 0$ for $\kappa$ and pass through the centres of the inclusions. The plots contain profiles for both level set reconstructions, the CG reconstruction, and the target distribution. It can be seen that the boundary localisation for both level set reconstructions, as well as the contrast for the combined shape and contrast reconstruction, are significantly superior to the voxel-based reconstruction which tends to smooth out the boundaries and underestimates the object contrast.

The evolution of the contrast in the level set reconstruction is shown in Fig. 4. The contrast levels were held fixed during the first 20 iterations. After that, both shape and contrast were updated in each iteration. It can be seen that both absorption and scattering contrast propagate towards their target levels, with diffusion contrast converging at a faster rate.

The objective function $J^{(k)}$ as a function of iteration index $k$ for both level set reconstructions and the CG reconstruction is shown in Fig. 5. The cost functions decrease at a similar rate for both level set cases. It is interesting to note that the objective function for the CG reconstruction decreases at a significantly higher rate.

The $L_2$ norms of the differences between target and reconstructed images as a function of
Figure 5. Objective functions for shape reconstruction and combined shape and contrast reconstruction as a function of iteration index. For comparison, the objective function for the voxel-based CG is also shown.

Figure 6. $L_2$ norms of image differences between reconstructed and target images as a function of iteration, for shape reconstruction and combined shape and contrast reconstruction, as a function of iteration. For comparison, the image errors for a voxel-based CG reconstruction are also shown. Left: absorption reconstruction, right: diffusion reconstruction.

iteration are shown in Fig. 6 for both level set reconstructions and the CG reconstruction. The level set image errors for shape reconstructions converge faster than those for the combined shape and contrast reconstruction. The image errors for both level set reconstructions compare favourably to the CG image errors, in marked contrast to the behaviour of the objective functions. In particular for the absorption reconstruction, level set reconstructions achieve a lower error norm.

3.2. Head model
A second test case employed a head-shaped mesh of dimensions $50 \times 60 \times 40$ mm, consisting of 8163 8-noded voxel elements and 9821 nodes. Mean background parameters were set to $\bar{\mu}_{bg} = 0.01$ mm$^{-1}$ and $\bar{\kappa}_{bg} = 0.33$ mm, and 3% Gaussian-distributed random noise was added to this homogeneous background. Into this background were inserted two spherical objects of
increased absorption coefficient of $\mu_{obj} = 0.02$ mm$^{-1}$, two objects of decreased diffusion coefficient $\kappa_{obj} = 0.165$ mm, and one object with increased absorption and decreased diffusion coefficient. The distribution of inclusions can be seen in Fig. 7.

40 sources and 40 detectors were placed in 4 rings of 10 sources and 10 detectors each around the top of the head. Complex exitance values of light transmission from sources modulated at 100 MHz were calculated for all 1600 source-detector combinations.

As in section 3.1, two sets of level set reconstructions were performed, one for shape reconstruction only, using the correct contrast values for the inclusions, and one for a combined shape and contrast reconstruction, starting from an initial guess for the inclusion contrasts of $\mu_{obj} = 0.015$ mm$^{-1}$ and $\kappa_{obj} = 0.22$ mm. The results of the reconstructions after 70 iterations are shown in Fig. 8. It can be seen that the locations and shape of the objects are well recovered, although some of the absorption objects are not well separated, and some noise is evident in the diffusion images. This could be caused by an insufficient density of boundary measurement positions.

The contrast evolution for the combined shape and contrast reconstruction is shown in Fig. 9. The diffusion contrast shows the correct trend but only achieves about one half of the required change. Absorption contrast shows very little change. As with the shape evolution, a higher data sampling density may improve the results.

4. Conclusions
We have demonstrated the application of a level set approach to simultaneous 3-D absorption and diffusion image reconstruction in optical tomography. This method reconstructs the shape and contrast of included objects on a constant or mildly varying background. Compared to reconstruction techniques that recover the parameters of individual voxels, this technique preserves sharp region edges and does not suffer from blurring and contrast degradation of small features. We have shown that for the recovery of multiple high-contrast absorption and diffusion objects, the level set techniques can perform better than a conjugate gradient reconstruction of a voxel image in terms of the achievable image errors. When the contrast of the inclusions is reconstructed in addition to the shapes, we found that object shapes are generally recovered at
Figure 8. Iso-surfaces of targets (green) and reconstructed absorption and diffusion objects (red) for the shape-only (top) and combined shape and contrast level-set reconstructions (bottom). Left images show absorption, right images show diffusion.

an early stage of the reconstruction, while the object contrast typically converges slower. The diffusion parameter converges faster than the absorption parameter.

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Figure 9. Contrast evolution for level set reconstruction of head mesh. Target contrasts are shown as dashed lines.

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