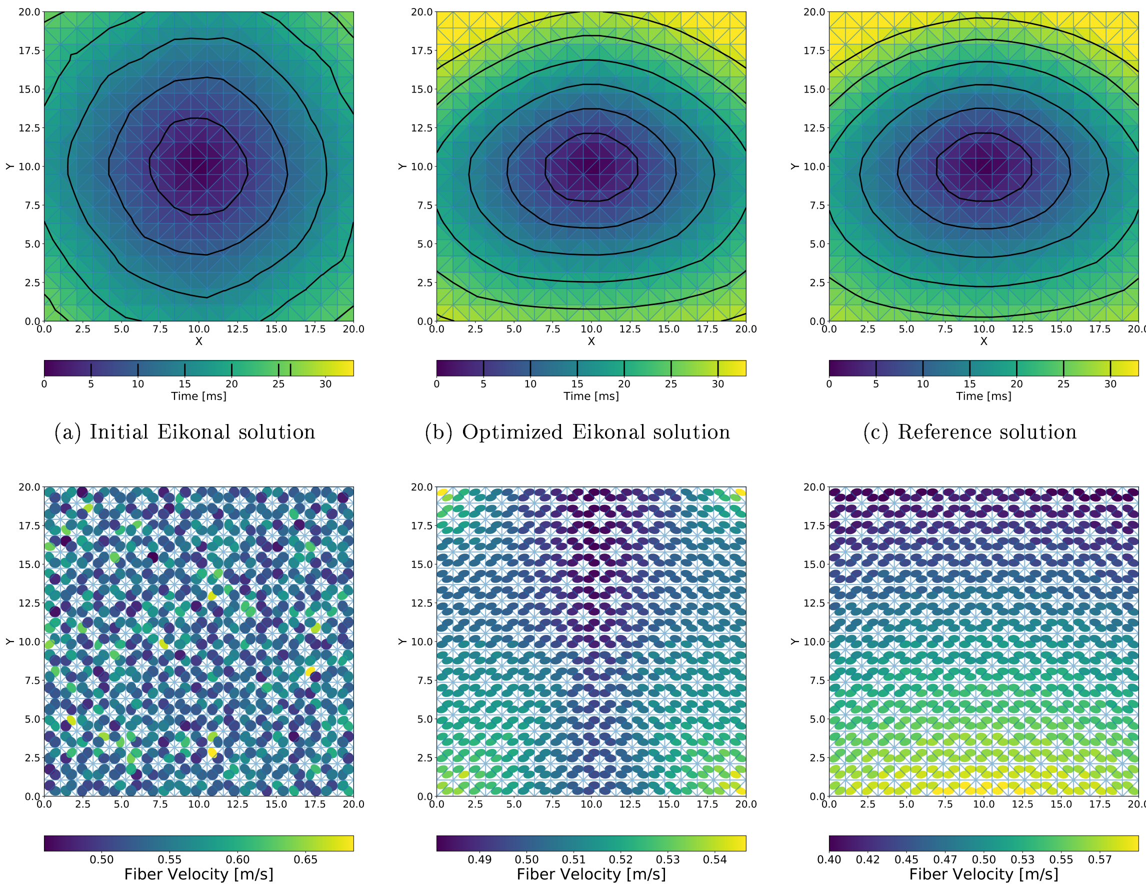
Appendix A Appendix

A.1 Additional 2D Experiments

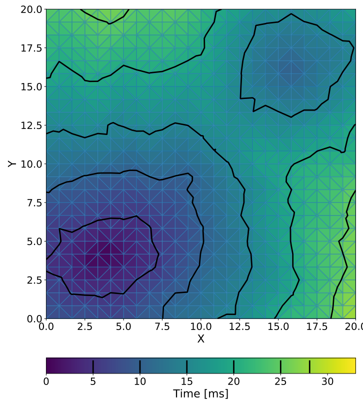


(a) Initial Eikonal solution (b) Optimized Eikonal solution (c) Reference solution

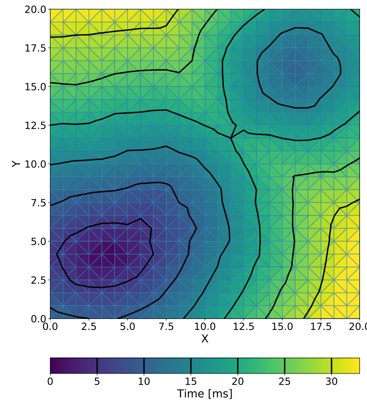
(d) Initial DTF (e) Optimized DTF (f) Reference DTF

Figure A1: This experiment uses curvature in horizontal direction, as well as a fiber velocity gradient along vertical direction. We are able to reconstruct the curvature of the DTF and some parts of the velocity gradients. The upper part of the domain has slightly too high fiber velocities, compensated by overall lower fiber velocity across the domain.

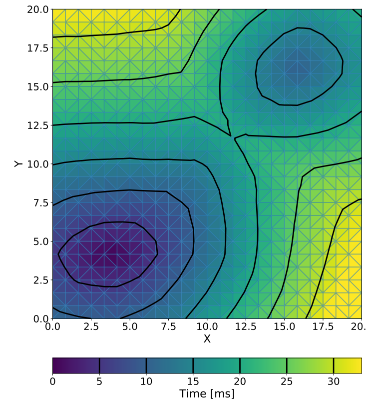
This section contains additional 2D experiments that demonstrate the results to be expected from the method presented in this paper. Fig. A1 is uses simple curvature of fiber, together with a velocity gradient in vertical direction, while Fig. A2 tries to reflect the joining of fibers in the heart's apex. Both examples can be reconstructed well from only boundary data, were the mismatch of activatoin times is close to zero, but there is some deviation in velocities and fiber direction, due to ill-posedness of the problem.



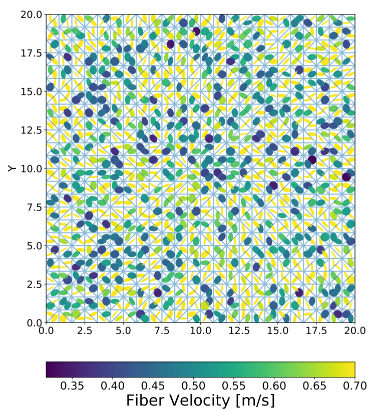
(a) Initial Eikonal solution



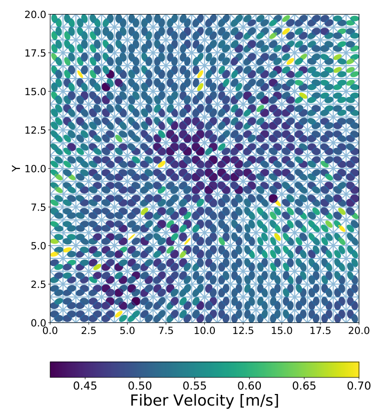
(b) Optimized Eikonal solution



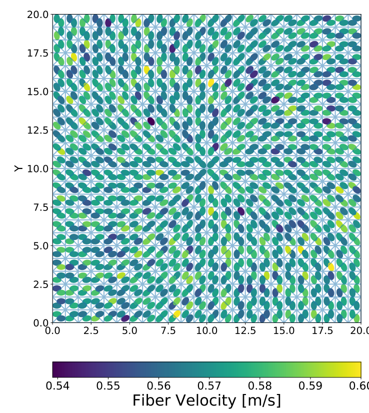
(c) Reference solution



(d) Initial DTF



(e) Optimized DTF



(f) Reference DTF

Figure A2: This experiment replicates a projection from below of the heart's apex: The fibers join in a circular fashion in the middle of the domain, fiber velocities are constant. Both fiber velocity and direction can be roughly reconstructed.

A.2 Optimal Choice of λ

This section will show how we arrive at the optimal choice of λ in Eq. (6). The used notation is a combination of the notations in [62] and [27], on which we based our solution to the problem. We start with our optimization problem, posed in Eq. (6):

$$\phi_4 = \min_{\lambda_1, \lambda_2} \lambda_1 \phi_1 + \lambda_2 \phi_2 + (1 - \lambda_1 - \lambda_2)\phi_3 + \sqrt{\mathbf{e}_\Delta^T D_j \mathbf{e}_\Delta}, \text{ s.t.: } \lambda_i \in [0, 1] \tag{25}$$

$$\begin{aligned} \mathbf{e}_\Delta &= \mathbf{v}_4 - \sum_{i=1}^{3} \lambda_i \mathbf{v}_i = \underbrace{\mathbf{v}_4 - \mathbf{v}_3}_{\mathbf{w}_3} + \lambda_1 \underbrace{(\mathbf{v}_3 - \mathbf{v}_1)}_{\mathbf{w}_1} + \lambda_2 \underbrace{(\mathbf{v}_3 - \mathbf{v}_2)}_{\mathbf{w}_2} \\ &= \lambda_1 \mathbf{w}_1 + \lambda_2 \mathbf{w}_2 + \mathbf{w}_3 \end{aligned} \tag{26}$$

where $\mathbf{v}_i \in \mathbb{R}^3$ are the vertices (corners) of our Tetrahedron. The wave propagation is calculated from the triangle formed by $(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$ to the vertex $\mathbf{v}_4$.

$$\begin{aligned}\phi_4 &= \min_{\lambda_1,\lambda_2} \lambda_1\phi_1 + \lambda_2\phi_2 + (1-\lambda_1-\lambda_2)\phi_3 + \sqrt{\mathbf{e}_\Delta^T D_j \mathbf{e}_\Delta} \\ &= \min_{\lambda_1,\lambda_2} \lambda_1(\phi_1-\phi_3) + \lambda_2(\phi_2-\phi_3) + \phi_3 + \|\lambda_1\mathbf{w}_1 + \lambda_2\mathbf{w}_2 + \mathbf{w}_3\|_{2,D}\end{aligned} \tag{27}$$

We state the unconstrained optimality condition as:

$$\begin{aligned}\nabla\phi_4 = \begin{pmatrix}\phi_1 - \phi_3 + \frac{1}{\|\mathbf{e}_\Delta\|}\mathbf{e}_\Delta^T D_j \mathbf{w}_1 \\ \phi_2 - \phi_3 + \frac{1}{\|\mathbf{e}_\Delta\|}\mathbf{e}_\Delta^T D_j \mathbf{w}_2\end{pmatrix} = \mathbf{0} \\ \mathbf{0} = \begin{pmatrix}(\phi_2-\phi_3)\|\mathbf{e}_\Delta\| + \frac{\phi_2-\phi_3}{\phi_1-\phi_3}\mathbf{e}_\Delta^T D_j \mathbf{w}_1 \\ (\phi_2-\phi_3)\|\mathbf{e}_{5,4}\| + \mathbf{e}_\Delta^T D_j \mathbf{w}_2\end{pmatrix}\end{aligned} \tag{28}$$

Subtract 1 from 2:

$$\begin{aligned}0 &= \mathbf{e}_\Delta^T D_j \left(\mathbf{w}_2 - \mathbf{w}_1\frac{\phi_2-\phi_3}{\phi_1-\phi_3}\right) \\ 0 &= (\lambda_1\mathbf{w}_1 + \lambda_2\mathbf{w}_2 + \mathbf{w}_3)^T D_j \left(\mathbf{w}_2 - \mathbf{w}_1\frac{\phi_2-\phi_3}{\phi_1-\phi_3}\right)\end{aligned} \tag{29}$$

For shorter notation, we write $r_{i,j} = \mathbf{w}_i^T D\mathbf{w}_j$. Since we require $D \in S_{++}^n$ (see Eq. (4)), $r_{i,j} = r_{j,i} \wedge r_{i,j} > 0$. Assume we want to find one of the lambda-variables, which we call λ_i, while the other λ will be called λ_k. We then have:

$$\begin{aligned}0 &= \lambda_1\Bigg(\underbrace{r_{1,2} - \frac{\phi_2-\phi_3}{\phi_1-\phi_3}r_{1,1}}_{A_1}\Bigg) + \lambda_2\Bigg(\underbrace{r_{2,2} - \frac{\phi_2-\phi_3}{\phi_1-\phi_3}r_{2,1}}_{A_2}\Bigg) + \underbrace{r_{3,2} - \frac{\phi_2-\phi_3}{\phi_1-\phi_3}r_{3,1}}_{B} \\ \lambda_k &= -\frac{B}{A_j} - \lambda_i\frac{A_i}{A_j}\end{aligned} \tag{30}$$

If either $A_1 = 0$ or $A_2 = 0$ are zero, the choice of λ_1 or λ_2 (respectively) is arbitrary. The solution for the variable with $A_i \neq 0$ is then $\lambda_i = -\frac{B}{A_i}$. For the general case $A_1 \neq 0$ and $A_2 \neq 0$ we reintroduce the solution of λ_k into the original minimization problem to find the optimal λ_i:

$$\begin{aligned}\lambda_i =& \arg\min_\lambda \lambda(\phi_i-\phi_3) + \lambda_k(\phi_j-\phi_3) + \phi_3 + \|\lambda\mathbf{w}_i + \lambda_k\mathbf{w}_j + \mathbf{w}_3\|_{2,D} \\ & \arg\min_\lambda \lambda(\phi_i-\phi_3) + \left(-\frac{B}{A_j} - \lambda\frac{A_i}{A_j}\right)(\phi_j-\phi_3) + \phi_3 + \left\|\lambda\mathbf{w}_i + \left(-\frac{B}{A_j} - \lambda\frac{A_i}{A_j}\right)\mathbf{w}_j + \mathbf{w}_3\right\|_{2,D} \\ & \arg\min_\lambda \lambda\left(\phi_i - \phi_3 - \frac{A_i}{A_j}(\phi_j-\phi_3)\right) - \frac{B}{A_j}(\phi_j-\phi_3) + \phi_3 + \Bigg\|\lambda\underbrace{\left(\mathbf{w}_i - \frac{A_i}{A_j}\mathbf{w}_j\right)}_{\mathbf{z}_1} + \underbrace{\mathbf{w}_3 - \frac{B}{A_j}\mathbf{w}_j}_{\mathbf{z}_2}\Bigg\|_{2,D}\end{aligned} \tag{31}$$

and solve the problem using the optimality condition again

$$\begin{aligned}
0 &= \left(\phi_i - \phi_3 - \frac{A_i}{A_j}\left(\phi_j - \phi_3\right)\right) + \frac{1}{\|\lambda \mathbf{z}_1 + \mathbf{z}_2\|_{2,D}} \mathbf{z}_1^T D \left(\lambda \mathbf{z}_1 + \mathbf{z}_2\right) \\
&= \left(\phi_i - \phi_3 - \frac{A_i}{A_j}\left(\phi_j - \phi_3\right)\right) \|\lambda \mathbf{z}_1 + \mathbf{z}_2\|_{2,D} + \lambda \mathbf{z}_1^T D \mathbf{z}_1 + \mathbf{z}_1^T D \mathbf{z}_2
\end{aligned} \tag{32}$$

We again write for a shorter notation $p_{i,j} = \mathbf{z}_i^T D \mathbf{z}_j$

$$\begin{aligned}
-\left(\phi_i - \phi_3 - \frac{A_i}{A_j}\left(\phi_j - \phi_3\right)\right) \|\lambda \mathbf{z}_1 + \mathbf{z}_2\|_{2,D} &= \lambda p_{1,1} + p_{1,2} \\
\underbrace{\left(\phi_i - \phi_3 - \frac{A_i}{A_j}\left(\phi_j - \phi_3\right)\right)^2}_{t} \left(\lambda^2 p_{1,1} + 2\lambda p_{1,2} + p_{2,2}\right) &= \lambda^2 p_{1,1}^2 + 2\lambda p_{1,1} p_{1,2} + p_{1,2}^2 \\
\lambda^2 \left(p_{1,1} t - p_{1,1}^2\right) + \lambda \left(2 p_{1,2} t - 2 p_{1,1} p_{1,2}\right) + p_{2,2} t - p_{1,2}^2 &= 0
\end{aligned} \tag{33}$$

The solution to the quadratic problem is

$$\begin{aligned}
\lambda_{1,2} &= \frac{-\left(2p_{1,2}t - 2p_{1,1}p_{1,2}\right) \pm \sqrt{4\left(p_{1,2}t - p_{1,1}p_{1,2}\right)^2 - 4\left(p_{1,1}t - p_{1,1}^2\right)\left(p_{2,2}t - p_{1,2}^2\right)}}{2\left(p_{1,1}t - p_{1,1}^2\right)} \\
&= \frac{-\left(t - p_{1,1}\right) p_{1,2} \pm \sqrt{p_{1,2}t^2 - p_{1,1}p_{1,2}^2 t - p_{1,1}p_{2,2}t^2 + p_{1,1}^2 p_{2,2} t}}{\left(t - p_{1,1}\right) p_{1,1}} \\
&= \frac{-p_{1,2} \pm \sqrt{\frac{1}{\left(t - p_{1,1}\right)^2} t \left(t - p_{1,1}\right)\left(p_{1,2}^2 - p_{1,1}p_{2,2}\right)}}{p_{1,1}} \\
&= \frac{-p_{1,2} \pm \sqrt{t \frac{p_{1,1}p_{2,2} - p_{1,2}^2}{p_{1,1} - t}}}{p_{1,1}} \\
&= \frac{-p_{1,2} \pm k \sqrt{\frac{p_{1,1}p_{2,2} - p_{1,2}^2}{p_{1,1} - t}}}{p_{1,1}}
\end{aligned} \tag{34}$$

with $k = \sqrt{t}$.

Both solutions need to be checked and the value that minimizes ϕ_4 in Eq. (25) is taken. λ_k is then easily obtained using Eq. (30).

Special cases may arise when solving Eq. (34) unconstrained as Fu et al. already stated:

> *If no root exists, or if λ_1 or λ_2 falls outside the range of $[0, 1]$ (that is, the characteristic direction does not reside within the tetrahedron), we then apply the 2D local solver used in [26] to the faces $\Delta_{1,2,4}$, $\Delta_{1,3,4}$ and $\Delta_{2,3,4}$ and select the minimal solution from among the three.* ([27])

The referenced 2D solver finds the optimal λ for the wave propagation in triangles through solving the following optimization problem:

$$\phi_3 = \min_{\lambda} \lambda\phi_1 + (1-\lambda)\phi_2 + \phi_3 + \sqrt{\mathbf{e}_{4,3}^T D_j \mathbf{e}_{4,3}}, \quad \text{s.t.: } \lambda \in [0,1] \tag{35}$$

with

$$\mathbf{e}_{4,3} = \mathbf{v}_3 - (\lambda\mathbf{v}_1 + (1-\lambda)\mathbf{v}_2) = \mathbf{v}_3 - \mathbf{v}_1 + \lambda(\mathbf{v}_2 - \mathbf{v}_1) \tag{36}$$

The derivation is similar to the presented 3D-case.

A.3 Gradient of λ

The optimization is kept as general as possible, by assuming that all variables, except the coordinates of the vertices, are dependant on our exemplary variable y. If we remember the minimizing sign in Eq. (34), we can state the solution of λ as:

$$\lambda = \frac{-p_{1,2}(y) + c\, k(y)\sqrt{\frac{p_{1,1}(y)p_{2,2}(y) - p_{1,2}(y)^2}{p_{1,1}(y) - t(y)}}}{p_{1,1}(y)} \quad \text{s.t.: } c \in \{-1, 1\} \tag{37}$$

In order to derive λ, we recall the definitions of all former temporary shorthand notations and their gradients. Additionally, some of the longer terms also receive their shorthand notation:

$$\begin{aligned} \mathbf{w}_i &= \mathbf{v}_3 - \mathbf{v}_i & \frac{\partial \mathbf{w}_i}{\partial y} &= \mathbf{0} \\ r_{i,j}(y) &= \mathbf{w}_i^T D(y)\mathbf{w}_j & \frac{\partial r_{i,j}(y)}{\partial y} &= \mathbf{w}_i^T \frac{\partial D(y)}{\partial y}\mathbf{w}_j \\ k_i(y) &= \phi_i(y) - \phi_3(y) & \frac{\partial k_i(y)}{\partial y} &= \frac{\partial \phi_i}{\partial y} - \frac{\partial \phi_3}{\partial y} \end{aligned} \tag{38}$$

$$\begin{aligned} A_i(y) &= k_1(y)r_{i,2}(y) - k_2(y)r_{i,1}(y) \\ \frac{\partial A_i}{\partial y} &= \frac{\partial k_1}{\partial y}r_{i,2}(y) + k_1(y)\frac{\partial r_{i,2}}{\partial y} - \frac{\partial k_2}{\partial y}r_{i,1}(y) - k_2(y)\frac{\partial r_{i,1}}{\partial y} \\ B &= k_1(y)r_{3,2}(y) - k_2(y)r_{3,1}(y) \\ \frac{\partial B}{\partial y} &= \frac{\partial k_1}{\partial y}r_{3,2}(y) + k_1(y)\frac{\partial r_{3,2}(y)}{\partial y} - \frac{\partial k_2}{\partial y}r_{3,1}(y) - k_2(y)\frac{\partial r_{3,1}(y)}{\partial y} \\ k(y) &= k_i(y) - \frac{A_i(y)}{A_j(y)}k_j(y) \\ \frac{\partial k}{\partial y} &= \frac{\partial k_i}{\partial y} - \left(\frac{\frac{\partial A_i}{\partial y}A_j(y) - A_i(y)\frac{\partial A_j}{\partial y}}{A_j(y)^2}k_j(y) + \frac{A_i(y)}{A_j(y)}\frac{\partial k_j}{\partial y} \right) \\ t(y) &= k(y)^2 \\ \frac{\partial t}{\partial y} &= 2k\frac{\partial k}{\partial y} \end{aligned} \tag{39}$$

$$
\begin{aligned}
\mathbf{z}_1(y) &= \mathbf{w}_i - \frac{A_i(y)}{A_j(y)}\mathbf{w}_j \\
\frac{\partial \mathbf{z}_1}{\partial y} &= \mathbf{w}_i - \left(\frac{\frac{\partial A_i}{\partial y}A_j(y) - A_i(y)\frac{\partial A_j}{\partial y}}{A_j(y)^2}\right)\mathbf{w}_j \\
\mathbf{z}_2(y) &= \mathbf{w}_3 - \frac{B(y)}{A_j(y)}\mathbf{w}_j \\
\frac{\partial \mathbf{z}_2}{\partial y} &= \mathbf{w}_3 - \left(\frac{\frac{\partial B}{\partial y}A_j(y) - B(y)\frac{\partial A_j}{\partial y}}{A_j(y)^2}\right)\mathbf{w}_j \\
p_{i,j}(y) &= \mathbf{z}_i^T(y)D(y)\mathbf{z}_j(y) \\
\frac{\partial p_{i,j}}{\partial y} &= \frac{\partial \mathbf{z}_i^T}{\partial y}D(y)\mathbf{z}_j(y) + \mathbf{z}_i^T(y)\frac{\partial D}{\partial y}\mathbf{z}_j(y) + \mathbf{z}_i^T(y)D(y)\frac{\partial \mathbf{z}_j}{\partial y}
\end{aligned}
\tag{40}
$$

Additionally we introduce a shorthand notation for the fraction of the square root in (37):

$$
\begin{aligned}
u(y) &= p_{1,1}p_{2,2} - p_{1,2}^2 \\
\frac{\partial u}{\partial y} &= \frac{\partial p_{1,1}}{\partial y}p_{2,2}(y) + p_{1,1}(y)\frac{\partial p_{2,2}}{\partial y} - 2p_{1,2}\frac{\partial p_{1,2}}{\partial y} \\
v(y) &= p_{1,1} - t \\
\frac{\partial v}{\partial y} &= \frac{\partial p_{1,1}}{\partial y} - \frac{\partial t}{\partial y}
\end{aligned}
\tag{41}
$$

Deriving Eq. (37) using the derivation of all shorthand variables yields the gradient of λ:

$$
\begin{aligned}
\lambda(y) =& \frac{p_{1,2}(y) + c\,k(y)\sqrt{\frac{u(y)}{v(y)}}}{p_{1,1}(y)} \\
\frac{\partial \lambda}{\partial y} =& \frac{1}{p_{1,1}(y)^2}\left[\left(\frac{\partial p_{1,2}}{\partial y} + c\left(\frac{\partial k}{\partial y}\sqrt{\frac{u(y)}{v(y)}} + \frac{1}{2}\sqrt{\frac{v(y)}{u(y)}}\frac{\frac{\partial u}{\partial y}v(y) - u(y)\frac{\partial v}{\partial y}}{v(y)^2}\right)\right)p_{1,1}(y) - \left(p_{1,2}(y) + c\,k(y)\sqrt{\frac{u(y)}{v(y)}}\right)\frac{\partial p_{1,1}}{\partial y}\right]
\end{aligned}
\tag{42}
$$

A.4 Gradient-Approximation of the Diffusion Tensors

We want to find ∇D given D on an unstructured grid. We know that for any closed domain $\omega \subset \Omega$, it holds that

$$
\int_\omega \nabla D(\mathbf{x})\,\mathrm{d}x = \int_{\partial\omega} D(\mathbf{x})\,\mathrm{d}x
$$

Assume our domain of interest ω encompasses exactly one element j. Since we assume constancy of gradient of diffusion tensors $\forall \mathbf{x} \in \omega : \nabla D(\mathbf{x}) = \nabla D_j$ inside one element, we can say that

$$|\omega| \nabla D_j = \int_{\partial\omega} D(\mathbf{x}) \,\mathrm{d}x$$

Our elements are not arbitrary domains, but are either triangles ($d = 3$) or tetrahedra ($d = 4$), with a finite set of linear lines/faces $\partial\omega_i$:

$$|\omega| \nabla D_j = \sum_{i=1}^{d} \int_{\partial\omega_i} D(\mathbf{x}) \,\mathrm{d}x$$

In order to compute the integral on the r.h.s., we need to define a proper function that approximates $D(\mathbf{x})$ on the faces. For our experiments, we computed the mean of elements sharing the face.

There are many sophisticated solutions to this problem, but we used the simple assumption that $D(\mathbf{x})$ is the constant mean on each face/line of all elements bordering the line/face. We use a von-Neumann boundary condition with zero flux outside of our domain for all surface faces $\omega_i \in \partial\Omega$.