# Weierstraß-Institut für Angewandte Analysis und Stochastik 

 Leibniz-Institut im Forschungsverbund Berlin e. V.
# Improved dual meshes using Hodge-optimized triangulations for electromagnetic problems 

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submitted: September 21, 2015

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No. 2156
Berlin 2015


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#### Abstract

Hodge-optimized triangulations (HOT) can optimize the dual mesh alone or both the primal and dual meshes. They make them more self-centered while keeping the primal-dual orthogonality. The weights are optimized in order to improve one or more of the discrete Hodge stars. Using the example of Maxwell's equations we consider academic examples to demonstrate the generality of the approach.


## 1 Introduction

First we start with the definition of a $k$-simplex. A $k$-simplex $\sigma^{k}$ is the convex hull of $k+1$ geometrically independent points $\mathbf{x}_{\mathbf{1}}, \ldots, \mathbf{x}_{\mathbf{k}+\mathbf{1}} \in \mathbb{R}^{d}$ with $d \in\{0,1,2,3\}$ and $0 \leq k \leq d$.

$$
\begin{equation*}
\sigma^{k}=\left\{\mathbf{z} \in \mathbb{R}^{d}: \mathbf{z}=\sum_{i=1}^{k+1} \lambda_{i} \mathbf{x}_{\mathbf{i}}, 0 \leq \lambda_{i} \leq 1, \sum_{i=1}^{k+1} \lambda_{i}=1\right\} \tag{1}
\end{equation*}
$$

Any simplex spanned by a proper subset of $\left\{\mathbf{x}_{\mathbf{1}}, \ldots, \mathbf{x}_{\mathbf{k}+\boldsymbol{1}}\right\}$ is called a face of $\sigma^{k}$. The union of the proper faces of $\sigma^{k}$ is called its boundary. The interior of $\sigma^{k}$ is the set difference of $\sigma^{k}$ and its boundary. The interior of $\sigma^{0}$ is $\sigma^{0}$. The volume of $\sigma^{k}$ is denoted by $\left|\sigma^{k}\right|$. Define $\left|\sigma^{0}\right|$ $=1$ (cf. [7]). Given a set of points $S \subset \mathbb{R}^{d}$. For $d=3$, the triangulation $\mathcal{T}(S)$ of this set of points is a set of tetrahedra (cf. [19]). Each $k$-simplex is associated with a dual $(d-k)$-cell, $* \sigma^{k}, k \in\{0,1,2,3\}$ (cf. [10]). The dual of $\mathcal{T}$ forms a cell complex $\mathcal{D}$. If the initial triangulation is Delaunay then this dual is simply the Voronoi diagram of the primal vertices. Thus, we obtain a primal-dual triangulation $(\mathcal{T}, \mathcal{D})$ with the nice properties of non-self-intersection, convexity, and orthogonality of the primal-dual elements (cf. [9]). The triangulations ( $\mathcal{T}, \mathcal{D}$ ) don't allow to change the dual mesh if the primary is fixed. The complex $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ is a generalization of $(\mathcal{T}, \mathcal{D})$ and provides orthogonal primal-dual triangulations with much more self-centered simplices $\sigma^{d}$. The regular triangulation $\mathcal{R} \mathcal{T}$ (weighted Delaunay triangulation) is a generalization of $\mathcal{T}$ and the power diagrams $\mathcal{P} \mathcal{D}$ (Laguerre or weighted Voronoi diagrams) are the dual structures of $\mathcal{R} \mathcal{T}$.

Each point $\mathbf{x}_{\mathbf{i}} \in \mathbb{R}^{d}$ in $\mathcal{R} \mathcal{T}$ is associated with a real number (weight) $w_{i} \in \mathbb{R}$ and $\left(\mathbf{x}_{\mathbf{i}}, w_{i}\right)$ is called as weighted point. The power distance of a point $\mathbf{z} \in \mathbb{R}^{d}$ with respect to a weighted point $\left(\mathbf{x}_{\mathbf{i}}, w_{i}\right)$ is defined as

$$
\begin{equation*}
\pi_{i}(\mathbf{z})=\left\|\mathbf{z}-\mathbf{x}_{\mathbf{i}}\right\|_{2}^{2}-w_{i} \tag{2}
\end{equation*}
$$

and it doesn't matter whether $\mathbf{z}$ is weighted or unweighted. Two weighted points ( $\mathbf{x}_{\mathbf{i}}, w_{i}$ ) and $\left(\mathbf{x}_{\mathbf{j}}, w_{j}\right)$ are said to be orthogonal if $\left\|\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{i}}\right\|^{2}=w_{i}+w_{j}$, i.e., $\pi_{i}\left(\mathbf{x}_{\mathbf{j}}\right)=w_{j}$. For each weighted point $\left(\mathbf{x}_{\mathbf{i}}, w_{i}\right)$ with $\mathbf{x}_{\mathbf{i}} \in S$, its power cell is defined by

$$
\begin{equation*}
\tilde{V}_{i}=\left\{\mathbf{z} \in \mathbb{R}^{d}: \pi_{i}(\mathbf{z}) \leq \pi_{j}(\mathbf{z}), \forall \mathbf{x}_{\mathbf{j}} \in S\right\} . \tag{3}
\end{equation*}
$$

More information on weighted Voronoi cells and the relation between regular triangulations in $\mathbb{R}^{d}$ and convex hulls in $\mathbb{R}^{d+1}$ can be found in $[9,13,19]$.

The weighted circumcenter, also called the orthogonal center, of a $k$-simplex $\sigma^{k}$ is computed by

$$
\begin{equation*}
\mathbf{c}\left(\sigma^{k}\right)=\mathbf{x}_{\mathbf{1}}+\frac{1}{2 k!\left|\sigma^{k}\right|} \sum_{\mathbf{x}_{\mathbf{j}} \in \sigma^{k}}\left(\left\|\mathbf{x}_{\mathbf{1}}-\mathbf{x}_{\mathbf{j}}\right\|^{2}+w_{l}-w_{j}\right) \hat{\mathbf{n}}_{\mathbf{j}}^{k} \tag{4}
\end{equation*}
$$

where $\mathbf{x}_{\mathbf{1}}$ is any of the vertices of $\sigma^{k}$ and $\hat{\mathbf{n}}_{\mathbf{j}}^{k}$ denotes the inward-pointing normal of the face of $\sigma^{k}$ opposite to $\mathbf{x}_{\mathbf{j}}$ (cf. [9]). For this, the orientation of the $d$-simplex $\sigma^{d}$, i.e., the orientation of the set of $d+1$ points is important. It is positive if the points occure in the orientation illustrated


Figure 1: A tetrahedron having positive orientation.
in Fig. 1. We can apply a right-hand rule: orient the right hand with fingers curled to follow the circular sequence $j k l$. If the thumb points toward $i$ then $\sigma^{d}$ has a positive orientation. In other words, the vectors $\mathbf{t}, \mathbf{u}$, and $\mathbf{v}$, in this order, define a positive frame. Using Eq. 4, we obtain for the orthogonal center $\mathbf{c}_{\mathrm{ijkl}}$ the following expression in $\mathbb{R}^{3}$ (cf. [13]):

$$
\begin{equation*}
\mathbf{c}_{\mathbf{i j k l}}=\mathbf{x}_{\mathbf{l}}+\frac{\left(\|\mathbf{t}\|^{2}+w_{l}-w_{i}\right) \hat{\mathbf{n}}_{\mathbf{i}}+\left(\|\mathbf{u}\|^{2}+w_{l}-w_{j}\right) \hat{\mathbf{n}}_{\mathbf{j}}+\left(\|\mathbf{v}\|^{2}+w_{l}-w_{k}\right) \hat{\mathbf{n}}_{\mathbf{k}}}{12\left|T_{i j k l}\right|} \tag{5}
\end{equation*}
$$

where $\left|T_{i j k l}\right|$ is the volume of the tetrahedron $T_{i j k l}$ spanned by the vertices $\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}, \mathbf{x}_{\mathbf{k}}$, and $\mathbf{x}_{\mathbf{1}}$. Using $\mathrm{t}=\mathrm{x}_{\mathrm{i}}-\mathrm{x}_{\mathrm{l}}, \mathbf{u}=\mathrm{x}_{\mathrm{j}}-\mathrm{x}_{\mathrm{l}}$, and $\mathrm{v}=\mathrm{x}_{\mathrm{k}}-\mathrm{x}_{1}$, the outward-pointing and inward-pointing normals are

$$
\begin{array}{rlrl}
\mathbf{n}_{\mathbf{i}} & =\mathbf{v} \times \mathbf{u}, & \hat{\mathbf{n}}_{\mathbf{i}} & =-\mathbf{n}_{\mathbf{i}}=\mathbf{u} \times \mathbf{v}, \\
\mathbf{n}_{\mathbf{j}} & =\mathbf{t} \times \mathbf{v}, & \hat{\mathbf{n}}_{\mathbf{j}}=-\mathbf{n}_{\mathbf{j}}=\mathbf{v} \times \mathbf{t}, \\
\mathbf{n}_{\mathrm{k}} & =\mathbf{u} \times \mathbf{t}, & \hat{\mathbf{n}}_{\mathbf{k}}=-\mathbf{n}_{\mathbf{k}}=\mathbf{t} \times \mathbf{u}, \quad \text { and } \\
\mathbf{n}_{\mathbf{l}} & =\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right) . & & \tag{6}
\end{array}
$$

An alternative formula for the last vector is $\mathbf{n}_{\mathbf{l}}=\hat{\mathbf{n}}_{\mathbf{i}}+\hat{\mathbf{n}}_{\mathbf{j}}+\hat{\mathbf{n}}_{\mathbf{k}}$. A simplex $\sigma^{k}$ is said to be self-centered if $\mathbf{c}\left(\sigma^{k}\right)$ lies in the interior of $\sigma^{k}$.

## 2 Hodge-optimized triangulations

For an arbitrary primal element $\sigma$, the diagonal approximation of the Hodge star of a continuous differential form $\alpha$ is given by the relation

$$
\begin{equation*}
\frac{1}{|* \sigma|} \int_{* \sigma} \star \alpha \approx \frac{1}{|\sigma|} \int_{\sigma} \alpha \tag{7}
\end{equation*}
$$

where $|\sigma|$ and $|* \sigma|$ are the volumes of these elements (cf. [9, 14]). Using Eq. (7) the error density $e_{i}$ on the dual of a $k$-simplex $\sigma_{i}^{k}$ is given as the average difference between the discrete approximation and the exact Hodge star:

$$
\begin{equation*}
e_{i}=\frac{1}{\left|* \sigma_{i}^{k}\right|}\left|\frac{\left|* \sigma_{i}^{k}\right|}{\left|\sigma_{i}^{k}\right|} \int_{\sigma_{i}^{k}} \alpha-\int_{* \sigma_{i}^{k}} \star \alpha\right|=\left|\frac{1}{\left|\sigma_{i}^{k}\right|} \int_{\sigma_{i}^{k}} \alpha-\frac{1}{\left|* \sigma_{i}^{k}\right|} \int_{* \sigma_{i}^{k}} \star \alpha\right| \tag{8}
\end{equation*}
$$

One can assemble a total error by summing the error densities $e_{i}$ over local regions, specific to $\sigma_{i}^{k}$ and $* \sigma_{i}^{k}$. These regions denoted as $\diamond\left(\sigma_{i}^{k} \cup * \sigma_{i}^{k}\right)$ are the convex hulls of $\sigma_{i}^{k}$ and $* \sigma_{i}^{k}$ (cf. [9, 10]).

$$
\begin{equation*}
E_{2}\left(\mathcal{R} \mathcal{T}, \mathcal{P D}, \star^{k}\right)=\left(\sum_{\sigma_{i}^{k}} \int_{\diamond\left(\sigma_{i}^{k} \cup * \sigma_{i}^{k}\right)} e_{i}^{2}\right)^{\frac{1}{2}}=\left(\sum_{\sigma_{i}^{k}} \frac{\left|\sigma_{i}^{k}\right|\left|* \sigma_{i}^{k}\right|}{\binom{d}{k}} e_{i}^{2}\right)^{\frac{1}{2}} \tag{9}
\end{equation*}
$$

Using the Wasserstein metric $W_{2}$ the following estimate is a useful bound of (9):

$$
\begin{equation*}
E_{2}\left(\mathcal{R} \mathcal{T}, \mathcal{P} \mathcal{D}, \star^{k}\right)^{2} \leq \frac{1}{\binom{d}{k}} \sum_{\sigma_{i}^{k}}\left|\sigma_{i}^{k}\right|\left|* \sigma_{i}^{k}\right| W_{2}\left(\sigma_{i}^{k}, * \sigma_{i}^{k}\right)^{2} \equiv \star^{k}-\mathrm{HOT}_{2,2}(\mathcal{R} \mathcal{T}, \mathcal{P} \mathcal{D}) \tag{10}
\end{equation*}
$$

### 2.1 General minimization procedure

A HOT mesh consists of a regular triangulation $\mathcal{R} \mathcal{T}$ and its associated power diagram $\mathcal{P D}$ for which $\mathcal{R} \mathcal{T}, \mathcal{P} \mathcal{D}$, or both have been optimized in order to reduce one HOT functional. A pseudocode of a general procedure is given in Table 1. This common minimization procedure works without anything else but an evaluation of a HOT energy and its gradient which will derive in closed form from direct integration.
Information about the solution of the unconstrained minimization problem

$$
\min _{\mathbf{x} \in \mathbb{R}^{n}} f(\mathbf{x})
$$

with the Wolfe conditions for some smooth $f: \mathbb{R}^{n} \longrightarrow \mathbb{R}$ can be found in [10]. The solution of the minimization problem occurs without updating the complex $(\mathcal{R} \mathcal{T}, \mathcal{P} \mathcal{D})$.

## $2.2 \mathrm{HOT}_{22}$ energies

The $\mathrm{HOT}_{2,2}$ energies can be expressed as a function of signed distances between the weighted circumcenters of $k$ - and $(k+1)$-simplices with $0 \leq k \leq d-1$ (cf. Fig. 2). The weighted

Table 1: Basic pseudocode of HOT mesh optimization.

```
Input: vertices \(\left\{\mathbf{x}_{\mathbf{i}}{ }^{0}\right\}\) with weights \(\mathbf{w}^{0}=\left\{w_{i}^{0}\right\}\) and
    \(0 \leq k \leq d\left(\right.\) type of \(\left.\star^{k}-\mathrm{HOT}_{2,2}(\mathcal{R} \mathcal{T}, \mathcal{P D})\right)\)
    Compute ( \(\mathcal{R} \mathcal{T}, \mathcal{P D}\) )
do \(m=1, \ldots, n_{w}\)
    Compute \(\star^{k}-\mathrm{HOT}_{2,2}(\mathcal{R T}, \mathcal{P D})\)
    do \(l=1, \ldots, n_{x}(m)\)
    Pick step direction \(\mathrm{d}_{x}\) for \(\star^{k}-\mathrm{HOT}_{2,2}(\mathcal{R T}, \mathcal{P D})\)
    Find \(\alpha\) satisfying Wolfe conditions
    \(\mathrm{x}_{\mathrm{i}}{ }^{l+1}:=\mathrm{x}_{\mathrm{i}}^{l}+\alpha \mathbf{d}_{x}\)
    Update ( \(\mathcal{R} \mathcal{T}, \mathcal{P D}\) )
    end ( \(l\) )
```

    Pick step direction \(\mathrm{d}_{w}\) for \(\star^{k}-\operatorname{HOT}_{2,2}(\mathcal{R} \mathcal{T}, \mathcal{P D})\)
    Find \(\beta\) satisfying Wolfe conditions
    \(\mathbf{w}^{m+1}:=\mathbf{w}^{m}+\beta \mathbf{d}_{w}\)
    Update \((\mathcal{R} \mathcal{T}, \mathcal{P D})\)
    end $(m)$
circumcenter of the $k$-simplex $\sigma^{k}$ is the orthogonal projection of the weigthted circumcenter of the ( $k+1$ )-simplex $\sigma^{k+1}$ onto simplex $\sigma^{k}$. The signed distance from the weighted circumcenter of $\sigma^{k+1}, c_{k+1}$, to the weighted circumcenter of $\sigma^{k}$ has a positive distance if the simplices $\sigma^{k+1}$ and $\left\{\sigma^{k}, c_{k+1}\right\}$ have the same orientation, and negative otherwise.
For both $\star^{0}$ and $\star^{d}$, $\mathrm{HOT}_{2,2}$ energies can be easily computed by splitting $d$-cells $* \sigma^{0}$ or primal $d$-simplices $\sigma^{d}$ into canonical subsimplices for which closed form integral expressions $W(\mathbf{p}, T)$ are found. $T$ is a tetrahedron spanned by the edges $a, b$, and $c$ and vertex $\mathbf{p}$ is adjacent to edge


Figure 2: Signed distances between circumcenters.
$a$ (cf. Fig. 2). Using the squared distance in Eq. (10) the integral expression $W(\mathbf{p}, T)$ is given by:

$$
\begin{equation*}
W(\mathbf{p}, T)=\int_{0}^{a} \int_{0}^{\frac{b}{a} x} \int_{0}^{\frac{c}{b} y}\left(x^{2}+y^{2}+z^{2}\right) d z d y d x=\frac{1}{5}\left(\frac{a^{3} b c}{2}+\frac{a b^{3} c}{4}+\frac{a b c^{3}}{12}\right) \tag{11}
\end{equation*}
$$

Using Eq. (11) and $\mathbf{p} \longleftarrow \mathbf{c}_{\mathbf{i j k l}}, a \longleftarrow H_{l(i j k)}, b \longleftarrow h_{k(i j)}$, and $c \longleftarrow d_{j(i)}$ the $\star^{3}-\mathrm{HOT}_{2,2}$ energy for every tetrahedron $T_{i j k l}$ is expressed as a function of the signed distances $d_{j(i)}$, $h_{k(i j)}$, and $H_{l(i j k)}$ between circumcenters as follows:

$$
\begin{aligned}
& \star^{3}-\mathrm{HOT}_{2,2}\left(T_{i j k l}\right)= \\
& \quad \sum_{r} \sum_{s} \sum_{t} \frac{1}{5}\left(\frac{H_{r(s t u)}^{3} h_{s(t u)} d_{t(u)}}{2}+\frac{H_{r(s t u)} h_{s(t u)}^{3} d_{t(u)}}{4}+\frac{H_{r(s t u)} h_{s(t u)} d_{t(u)}^{3}}{12}\right)
\end{aligned}
$$

where the indices $r, s, t$, and $u$ are determined by $r \in\{i, j, k, l\}, s \in\{i, j, k, l\} \backslash\{r\}$, $t \in\{i, j, k, l\} \backslash\{r, s\}$, and $u \in\{i, j, k, l\} \backslash\{r, s, t\}$. The arrangement of the indices $s, t$, and $u$ of $H_{r(s t u)}$ and $t$ and $u$ of $h_{s(t u)}$, respectively is not of any importance. Every permutation of $\{s, t, u\}$ yields the same distance $H_{r(\ldots)}$. The same applies to $\{t, u\}$ and $h_{s(\ldots)}$.
Thus, the total error (10) is computed by

$$
E_{2}\left(\mathcal{R T}, \mathcal{P D}, \star^{3}\right)^{2}=\sum_{T_{i j k l}} \star^{3}-\mathrm{HOT}_{2,2}\left(T_{i j k l}\right)
$$

Detailed information to the other remaining stars can be found in [10].
The signed distances $d_{j(i)}, h_{k(i j)}$, and $H_{l(i j k)}$ between (weighted) circumcenters $\mathbf{c}_{\mathbf{i}}\left(=\mathbf{x}_{\mathbf{i}}\right)$ and $\mathrm{c}_{\mathrm{ij}}, \mathrm{c}_{\mathrm{ij}}$ and $\mathrm{c}_{\mathrm{ijk}}$, and $\mathrm{c}_{\mathrm{ijk}}$ and $\mathrm{c}_{\mathrm{ijkl}}$ are given by (cf. [9, 10]):

$$
\begin{align*}
d_{j(i)} & =\frac{\ell_{i j}^{2}+w_{i}-w_{j}}{2 \ell_{i j}}, \quad \ell_{i j}=\left\|x_{j}-x_{i}\right\|  \tag{12a}\\
h_{k(i j)} & =\frac{\ell_{i j} \cot \gamma_{k}}{2}+\frac{w_{j} \cot \gamma_{i}+w_{i} \cot \gamma_{j}}{2 \ell_{i j}}-\frac{w_{k} \ell_{i j}}{4\left|t_{i j k}\right|}  \tag{12b}\\
H_{l(i j k)} & =\left(\mathbf{c}_{\mathbf{i j k}}-\mathbf{c}_{\mathbf{i j k l}}\right) \cdot \frac{\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)}{\left\|\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)\right\|}  \tag{12c}\\
& =\left\{\begin{array}{cl}
\left\|\mathbf{c}_{\mathbf{i j k}}-\mathbf{c}_{\mathbf{i j k} \mathbf{l}}\right\| & \text { if } \mathbf{x}_{\mathbf{l}} \text { and } \mathbf{c}_{\mathbf{i j k l}} \text { lie in the same half-plane } \\
-\left\|\mathbf{c}_{\mathbf{i j k}}-\mathbf{c}_{\mathbf{i j k} \mathbf{l}}\right\| & \text { otherwise } .
\end{array}\right. \tag{12d}
\end{align*}
$$

$\gamma_{i}$ is the angle at $\mathbf{x}_{\mathbf{i}}$ in triangle $t_{i j k}$ spanned by the vertices $\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}$, and $\mathbf{x}_{\mathbf{k}}$.

### 2.2.1 Weight optimization

The weight optimization of each $\mathrm{HOT}_{2,2}$ energy can easily done using the derivatives of Eq. (12):

$$
\frac{\partial d_{j(i)}}{\partial w_{i}}=\frac{1}{2 \ell_{i j}}, \quad \frac{\partial d_{j(i)}}{\partial w_{j}}=-\frac{1}{2 \ell_{i j}},
$$

$$
\begin{aligned}
\frac{\partial h_{k(i j)}}{\partial w_{i}} & =\frac{\cot \gamma_{j}}{2 \ell_{i j}}, \quad \frac{\partial h_{k(i j)}}{\partial w_{j}}=\frac{\cot \gamma_{i}}{2 \ell_{i j}}, \quad \frac{\partial h_{k(i j)}}{\partial w_{k}}=-\frac{\ell_{i j}}{4\left|t_{i j k}\right|} \\
\frac{\partial H_{l(i j k)}}{\partial w_{s}} & =\left(\frac{\partial \mathbf{c}_{\mathbf{i j k}}}{\partial w_{s}}-\frac{\partial \mathbf{c}_{\mathbf{i j k} \mathbf{k}}}{\partial w_{s}}\right) \cdot \frac{\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)}{\left\|\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)\right\|} \\
& =-\frac{1}{12\left|T_{i j k l}\right|} \mathbf{n}_{\mathbf{s}}^{3} \cdot \frac{\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)}{\left\|\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)\right\|} \\
& =\mp \frac{1}{12\left|T_{i j k l}\right|} \mathbf{n}_{\mathbf{s}}^{3} \cdot \frac{\left(\mathbf{c}_{\mathbf{i j k}}-\mathbf{c}_{\mathbf{i j k l} \mathbf{l}}\right)}{\left\|\mathbf{c}_{\mathbf{i j k}}-\mathbf{c}_{\mathbf{i j k l} \mid}\right\|}, \quad s \in\{i, j, k, l\}
\end{aligned}
$$

The derivative of the weighted circumcenter with respect to the weights at vertex $\mathrm{x}_{1}$ result in

$$
\frac{\partial \mathbf{c}_{\mathbf{i j k}}}{\partial w_{r}}=\frac{1}{4\left|t_{i j k}\right|} \mathbf{n}_{\mathbf{r}}^{2}, \quad \frac{\partial \mathbf{c}_{\mathbf{i j k}}}{\partial w_{l}} \equiv 0, \quad \text { and } \quad \frac{\partial \mathbf{c}_{\mathbf{i j k}}}{\partial w_{s}}=\frac{1}{12\left|T_{i j k l}\right|} \mathbf{n}_{\mathbf{s}}^{3}
$$

where $r \in\{i, j, k\}, s \in\{i, j, k, l\}$, and $\mathbf{n}_{\mathbf{r}}^{2}$ and $\mathbf{n}_{\mathbf{s}}^{3}$ denote the outward normals of the triangle $t_{i j k}$ and of the tetrahedron $T_{i j k l}$, respectively. The normal $\frac{\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)}{\left\|\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)\right\|}$ is perpendicular to $\mathbf{n}_{\mathrm{r}}^{2}$. The same applies for the normal $\frac{\left(c_{\mathrm{ijk}}-\mathrm{c}_{\mathbf{i j k}}\right)}{\left\|\mathrm{c}_{\mathrm{ijk}}-\mathrm{c}_{\mathrm{ijk}}\right\|} \|$.

### 2.2.2 Vertex position optimization

The derivatives of the signed distances between (weighted) circumcenters with respect to the vertices for Eq. (12a) are given by

$$
\begin{aligned}
\frac{\partial d_{j(i)}}{\partial \mathbf{x}_{\mathbf{i}}} & =\frac{\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{i}}\right)^{T}}{2}\left(\frac{w_{i}-w_{j}}{\ell_{i j}^{3}}-\frac{1}{\ell_{i j}}\right) \quad \text { and } \\
\frac{\partial d_{j(i)}}{\partial \mathbf{x}_{\mathbf{j}}} & =\frac{\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{i}}\right)^{T}}{2}\left(\frac{1}{\ell_{i j}}-\frac{w_{i}-w_{j}}{\ell_{i j}^{3}}\right)=-\frac{\partial d_{j(i)}}{\partial \mathbf{x}_{\mathbf{i}}} .
\end{aligned}
$$

Using Phytagoras' theorem, one can differentiate the signed distance $h_{k(i j)}$ (12b) between circumcenters $\mathrm{c}_{\mathrm{ij}}$ and $\mathrm{c}_{\mathrm{ijk}}$ in a triangle $t_{i j k}$ with respect to $\mathrm{x}_{\mathbf{i}}$.

$$
\begin{aligned}
\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j k}}\right\|^{2} & =\left\|\mathbf{c}_{\mathbf{i} \mathbf{j}}-\mathbf{c}_{\mathbf{i j k}}\right\|^{2}+\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i} \mathbf{j}}\right\|^{2} \\
h_{k(i j)}^{2} & =\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j k}}\right\|^{2}-d_{j(i)}^{2} \\
\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j k}} & =\frac{1}{4\left|t_{i j k}\right|} \sum_{r \in\{j, k\}}\left(\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{r}}\right\|^{2}+w_{i}-w_{r}\right) \mathbf{n}_{\mathbf{r}}^{2} \quad \text { by (4) }
\end{aligned}
$$

For the triangle $t_{i j k}$ with $\left|t_{i j k}\right|=\frac{1}{2}\left\|\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}}\right) \times\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right)\right\|$ we get

$$
\frac{\partial\left|t_{i j k}\right|}{\partial \mathbf{x}_{\mathbf{i}}}=\frac{1}{4\left|t_{i j k}\right|}\left(\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}}\right) \times\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right)\right)^{T} \cdot\left(I \times\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right)\right) .
$$

We finally obtain the following expression:

$$
\begin{equation*}
\frac{\partial h_{k(i j)}}{\partial \mathbf{x}_{\mathbf{i}}}=\frac{1}{h_{k(i j)}}\left(\left(\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j} \mathbf{k}}\right)^{T} \frac{\partial\left(\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j k}}\right)}{\partial \mathbf{x}_{\mathbf{i}}}-d_{j(i)} \frac{\partial d_{j(i)}}{\partial \mathbf{x}_{\mathbf{i}}}\right) . \tag{13}
\end{equation*}
$$

Similar formulas as Eq. (13) can be derived for $\frac{\partial h_{k(i j)}}{\partial \mathbf{x}_{\mathbf{j}}}$ and $\frac{\partial h_{k(i j)}}{\partial \mathbf{x}_{\mathbf{k}}}$, respectively.
Using Phytagoras' theorem twice, one can differentiate the signed distance $H_{l(i j k)}$ (12c),(12d) between circumcenters $\mathbf{c}_{\mathbf{i j k}}$ and $\mathbf{c}_{\mathbf{i j k l}}$ in a tetrahedron $T_{i j k l}$ with respect to $\mathbf{x}_{\mathbf{i}}$.

$$
\begin{aligned}
\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j k} \mathbf{k}}\right\|^{2} & =\left\|\mathbf{c}_{\mathbf{i j k}}-\mathbf{c}_{\mathbf{i j k} \mathbf{k}}\right\|^{2}+\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j k}}\right\|^{2} \\
& =\left\|\mathbf{c}_{\mathbf{i j k}}-\mathbf{c}_{\mathbf{i j k} \mathbf{k}}\right\|^{2}+\left\|\mathbf{c}_{\mathbf{i j}}-\mathbf{c}_{\mathbf{i j k}}\right\|^{2}+\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i} \mathbf{j}}\right\|^{2} \\
H_{l(i j k)}^{2} & =\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j k} \mathbf{l}}\right\|^{2}-\left(h_{k(i j)}^{2}+d_{j(i)}^{2}\right) \\
\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j k} \mathbf{l}} & =\frac{1}{12\left|T_{i j k l}\right|} \sum_{r \in\{j, k, l\}}\left(\left\|\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{r}}\right\|^{2}+w_{i}-w_{r}\right) \mathbf{n}_{\mathbf{r}}{ }^{2} \quad \text { by (4) }
\end{aligned}
$$

For the tetrahedron $T_{i j k l}$ with $\left|T_{i j k l}\right|=\frac{1}{6}\left|\left(\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}}\right) \times\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right)\right) \cdot\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{1}}\right)\right|$ we get

$$
\begin{aligned}
\frac{\partial\left|T_{i j k l}\right|}{\partial \mathbf{x}_{\mathbf{i}}}=\frac{1}{6} \frac{\left(\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}}\right) \times\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right)\right) \cdot\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{l}}\right)}{\left|\left(\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}}\right) \times\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right)\right) \cdot\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{l}}\right)\right|} \\
\quad\left(\left(\left(\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{k}}\right) \times\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{l}}\right)\right)^{T}+\left(\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}}\right) \times\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{k}}\right)\right)^{T}\right) .
\end{aligned}
$$

We finally obtain the following expression:

$$
\begin{equation*}
\frac{\partial H_{l(i j k)}}{\partial \mathbf{x}_{\mathbf{i}}}=\frac{1}{H_{l(i j k)}}\left(\left(\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i} \mathbf{j} \mathbf{k} \mathbf{l}}\right)^{T} \frac{\partial\left(\mathbf{x}_{\mathbf{i}}-\mathbf{c}_{\mathbf{i j} \mathbf{k} \mathbf{1}}\right)}{\partial \mathbf{x}_{\mathbf{i}}}-\left(h_{k(i j)} \frac{\partial h_{k(i j)}}{\partial \mathbf{x}_{\mathbf{i}}}+d_{j(i)} \frac{\partial d_{j(i)}}{\partial \mathbf{x}_{\mathbf{i}}}\right)\right) . \tag{14}
\end{equation*}
$$

Similar formulas as Eq. (14) can be derived for $\frac{\partial H_{l(i j k)}}{\partial \mathbf{x}_{\mathbf{j}}}, \frac{\partial H_{l(i j k)}}{\partial \mathbf{x}_{\mathbf{k}}}$, and $\frac{\partial H_{l(i j k)}}{\partial \mathbf{x}_{\mathbf{1}}}$.

## 3 Maxwellian grid equations

We consider the Maxwell's equations in integral form. We obtain in vector notation the following equations:

$$
\begin{align*}
\oint_{P} \mathbf{E} \cdot \mathrm{~d} \mathbf{l}=-\frac{\partial}{\partial t} \iint_{A} \mathbf{B} \cdot \mathrm{~d} \mathbf{A} & \oint_{P} \mathbf{H} \cdot \mathrm{~d} \mathbf{l}=\frac{\partial}{\partial t} \iint_{A} \mathbf{D} \cdot \mathrm{~d} \mathbf{A}+\iint_{A} \mathbf{J} \cdot \mathrm{~d} \mathbf{A} \\
\oiint_{S} \mathbf{B} \cdot \mathrm{~d} \mathbf{S}=0 & \oiint_{S} \mathbf{D} \cdot \mathrm{~d} \mathbf{S}=\iiint_{V} q \mathrm{~d} V . \tag{15}
\end{align*}
$$

The constitutive relations belonging to them are

$$
\begin{equation*}
\mathbf{D}=\varepsilon \mathbf{E}, \quad \mathbf{B}=\mu \mathbf{H}, \quad \mathbf{J}=\kappa \mathbf{E} . \tag{16}
\end{equation*}
$$

Here, $A$ is a surface with boundary curve $P, V$ is a volume bounded by a surface $S$, and $q$ is the volume charge density.

### 3.1 Discretization of Maxwell's equations

Given a set $S \subset \mathbb{R}^{3}$ of $n_{p}$ points $\mathbf{x}_{\mathbf{i}}=\sigma_{i}^{0}, i=1, \ldots, n_{p}$, and associated weights $w_{i} \in \mathbb{R}$. The regular triangulation $\mathcal{R} \mathcal{T}(S)$ consists of $n_{r} 3$-simplices (tetrahedra) $\sigma_{i}^{3}, i=1, \ldots, n_{r}, n_{f}$ faces $A_{i}=\sigma_{i}^{2}, i=1, \ldots, n_{f}$, and $n_{e}$ edges $L_{i}=\sigma_{i}^{1}, i=1, \ldots, n_{e}$. The power diagram $\mathcal{P D}$ consists of $n_{r} 0$-cells, $* \sigma_{i}^{3}$, i.e., the weighted orthogonal centers of $\sigma_{i}^{3}$, of $n_{f}$ edges $\tilde{L}_{i}$, $* \sigma_{i}^{2}, n_{e}$ faces $\tilde{A}_{i}, * \sigma_{i}^{1}$, and $n_{p} 3$-cells, $* \sigma_{i}^{0}$.
Using FIT [16, 17, $8,3,4,5,10$ ], the electric and magnetic voltages and fluxes over the elemtary objects of $\sigma_{i}^{3}$ and $* \sigma_{i}^{0}$ are defined as state variables in the following way:

$$
\begin{array}{rlr}
e_{i}=\int & h_{j}=\iint_{\tilde{L}_{j}} \mathbf{E} \cdot \mathrm{~d} \mathbf{l} \cdot \mathrm{~d} \mathbf{l} & i=1, \ldots, n_{e} \\
d_{i}=\iint_{\tilde{A}_{i}} \mathbf{D} \cdot \mathbf{n} \mathrm{~d} \mathbf{A} & b_{j}=\iint_{A_{j}} \mathbf{B} \cdot \mathbf{n} \mathrm{~d} \mathbf{A} & j=1, \ldots, n_{f} \\
j_{i}=\iint_{\tilde{A}_{i}} \mathbf{J} \cdot \mathbf{n} \mathrm{~d} \mathbf{A} & q_{k}=\iiint_{\tilde{V}_{k}} q \mathrm{~d} V & k=1, \ldots, n_{p}
\end{array}
$$

where $\mathbf{n}$ is the outward-pointing normal of the faces $A_{j}$ and $\tilde{A}_{i}$, respectively. The Maxwell's equations (cf. (15)) can then discretized for all the components [18]. Thus, we obtain a compact matrix-vector form:

$$
\begin{array}{ll}
C \mathbf{e}=-\frac{d}{d t} \mathbf{b}, & \tilde{C} \mathbf{h}=\frac{d}{d t} \mathbf{d}+\mathbf{j},  \tag{17}\\
S \mathbf{b}=0, & \tilde{S} \mathbf{d}=\mathbf{q}
\end{array}
$$

The matrices $C, C:=\left(c_{i j}\right)_{n_{f} \times n_{e}}$, and $\tilde{C}, \tilde{C}:=\left(\tilde{c}_{i j}\right)_{n_{e} \times n_{f}}$, represent the incidence relations between edges and faces on $\mathcal{R T}$ and $\mathcal{P D}$, respectively. Analogously, the matrices $S, S:=$ $\left(s_{i j}\right)_{n_{r} \times n_{f}}$, and $\tilde{S}, \tilde{S}:=\left(\tilde{s}_{i j}\right)_{n_{p} \times n_{e}}$, represent the incidence relations between faces and volumes on $\mathcal{R} \mathcal{T}$ and $\mathcal{P D}$, respectively. The matrices $C, \tilde{C}, S$, and $\tilde{S}$ satisfy the important relations

$$
\tilde{C}=C^{T}, \quad S C=0, \quad \text { and } \quad \tilde{S} \tilde{C}=0
$$

### 3.2 Discretization of the constitutive relations

To complete the system of equations (17), the quantities defined on the primary grid and the quantities defined on the dual grid are connected by the Hodge star operator, $\star$, (cf. [3, 15]):

$$
\begin{equation*}
D=\varepsilon \star E, \quad B=\mu \star H, \quad J=\kappa \star E . \tag{18}
\end{equation*}
$$

The Hodge operator depends on a metric. If the metric is taken to be the permittivity, the permeability, or the conductivity tensor, the constitutive relations (18) become

$$
\begin{equation*}
D=M_{\varepsilon} E, \quad B=M_{\mu} H, \quad J=M_{\kappa} E . \tag{19}
\end{equation*}
$$

Let $\sigma_{i}^{k}$ be the $i$-th $k$-simplex and $* \sigma_{i}^{k}$ the dual $(d-k)$-cell of the primal-dual triangulation $(\mathcal{R} \mathcal{T}, \mathcal{P D})$. Then the discrete $k$-th Hodge star is a diagonal matrix $M^{k}$ with

$$
\begin{equation*}
\left(M^{k}\right)_{i j}=\frac{\left|* \sigma_{i}^{k}\right|}{\left|\sigma_{i}^{k}\right|} \delta_{i j}, \quad \forall i, \forall j \tag{20}
\end{equation*}
$$

Thus, using (20) we get

$$
\begin{equation*}
\left(M_{\varepsilon}\right)_{i i}=\frac{\bar{\varepsilon} \tilde{A}_{i}}{L_{i}}, \quad\left(M_{\nu}\right)_{i i}=\frac{\bar{\nu} \tilde{L}_{i}}{A_{i}}, \quad \text { and } \quad\left(M_{\kappa}\right)_{i i}=\frac{\bar{\kappa} \tilde{A}_{i}}{L_{i}}, \tag{21}
\end{equation*}
$$

where $\bar{\varepsilon}$ is the face-averaged permittivity, $\bar{\nu}$ the edge-averaged reluctivity ( $\nu=\mu^{-1}$ ), and $\bar{\kappa}$ the face-averaged conductivity. If the weighted circumcenter of any simplex $\sigma_{i}^{d}$ is outside the simplex, i.e., $\sigma_{i}^{d}$ is not self-centered, then the matrices $M_{\varepsilon}, M_{\nu}$, and $M_{\kappa}$ (cf. (21)) are not positive definite. This is an important disadvantage.
For each simplex $\sigma_{i}^{d}$ that is not self-centered we use a locally barycentric dual mesh to make the matrices $M_{\varepsilon}, M_{\nu}$, and $M_{\kappa}$ symmetric positive definite. The construction of the constitutive matrices is performed using the microcell method (cf. [5, 10]). Microcells are elementary cells with hexahedral shape in the 3d cases. Each primary tetrahedral cell is divided by the dual edges in four different microcells, one for each of its four nodes (cf. [10]). The interpolation method starts from the assumption of a homogeneous medium and a constant field in the microcells (cf. [4, 5]). The global matrices $M_{\varepsilon}, M_{\nu}$, and $M_{\kappa}$ can be assembled from associated local matrices of the microcells (cf. [10]).
Another more widely used approach for barycentric dual meshes employs Whitney forms in the definition of the discrete Hodge star. Whitney $k$-forms are piecewise linear functions on a primal mesh. For a tetrahedron (Fig. 1), we use ordered indexing of nodes to denote the vertices (e.g. $\sigma^{0}=\left[\mathbf{x}_{\mathbf{i}}\right]$ ), oriented edges (e.g. $\sigma^{1}=\left[\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}\right]$ ), oriented faces (e.g. $\sigma^{2}=\left[\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}, \mathrm{x}_{\mathbf{k}}\right]$ ), and oriented cells (e.g. $\sigma^{3}=\left[\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}, \mathbf{x}_{\mathbf{k}}, \mathbf{x}_{\mathbf{1}}\right]$ ). In terms of vector proxies (cf. [3]), we have

$$
\begin{array}{ll}
\eta_{\sigma^{0}}=\lambda_{i} & \text { (Whitney 0-form) } \\
\eta_{\sigma^{1}}=\lambda_{i} \nabla \lambda_{j}-\lambda_{j} \nabla \lambda_{i} & \text { (Whitney 1-form) } \\
\eta_{\sigma^{2}}=2\left(\lambda_{i} \nabla \lambda_{j} \times \nabla \lambda_{k}+\lambda_{j} \nabla \lambda_{k} \times \nabla \lambda_{i}+\lambda_{k} \nabla \lambda_{i} \times \nabla \lambda_{j}\right) & \text { (Whitney 2-form) }  \tag{22}\\
\eta_{\sigma^{3}}=1 /\left|\sigma^{3}\right| \text { on } \sigma^{3}, 0 \text { elsewhere } & \text { (Whitney 3-form) }
\end{array}
$$

where $\lambda_{i}$ (cf. Eq. (1)) is the barycentric function for the vertex, i.e., $\lambda_{i}\left(\mathbf{x}_{\mathbf{j}}\right)=\delta_{i j}$. Using (22), we obtain

$$
\begin{equation*}
\left(M^{k, W h i t}\right)_{i j}=\int_{\Omega} \eta_{\sigma_{i}^{k}} \cdot \eta_{\sigma_{j}^{k}} d V . \tag{23}
\end{equation*}
$$

$M^{k, W h i t}$ is called the Galerkin Hodge. On a locally barycentric dual mesh we use Galerkin Hodges (23) based on Whitney edge and face elements on tetrahedron to obtain analogous formulas as (21):

$$
\begin{align*}
& \left(M_{\varepsilon}^{W h i t}\right)_{i j}=\int_{\Omega} \varepsilon \eta_{\sigma_{i}^{1}} \cdot \eta_{\sigma_{j}^{1}} d V, \quad\left(M_{\nu}^{W h i t}\right)_{i j}=\int_{\Omega} \nu \eta_{\sigma_{i}^{2}} \cdot \eta_{\sigma_{j}^{2}} d V  \tag{24}\\
& \left(M_{\kappa}^{W h i t}\right)_{i j}=\int_{\Omega} \kappa \eta_{\sigma_{i}^{1}} \cdot \eta_{\sigma_{j}^{1}} d V
\end{align*}
$$

### 3.3 Linear algebraic equations in the frequency domain

From Sec. 3.1, the equation for the fast varying transient electromagnetic fields is

$$
C^{T} M_{\nu} C \mathbf{e}+M_{\kappa} \frac{d}{d t} \mathbf{e}+M_{\varepsilon} \frac{d^{2}}{d t^{2}} \mathbf{e}=0
$$

If all field quantities vary sinusoidally with time, with angular frequency $\omega$, the electric field $\mathbf{E}(r, t)$ may be written as:

$$
\mathbf{E}(r, t)=\Re\left(\underline{\mathbf{E}(r)} e^{\jmath \omega t}\right)
$$

We get Maxwell's equations in phasor form:

$$
\begin{align*}
C \underline{\mathbf{e}} & =-\jmath \omega \underline{\mathbf{b}}  \tag{25}\\
C^{T} M_{\nu} \underline{\mathbf{b}} & =\jmath \omega M_{\varepsilon} \underline{\mathbf{e}}+M_{\kappa} \underline{\mathbf{e}} .
\end{align*}
$$

We obtain the eigenvalue problem

$$
C^{T} M_{\nu} C \underline{\mathbf{e}}+\jmath \omega M_{\kappa} \underline{\mathbf{e}}=\omega^{2} M_{\varepsilon} \underline{\mathbf{e}}
$$

and without lossy materials $\left(M_{\kappa}=0\right)$ the problem

$$
C^{T} M_{\nu} C \underline{\mathbf{e}}=\omega^{2} M_{\varepsilon} \underline{\mathbf{e}}
$$

Using

$$
\underbrace{\tilde{S} C^{T}}_{=0} M_{\nu} C \underline{\mathbf{e}}=\omega^{2} \tilde{S} M_{\varepsilon} \underline{\mathbf{e}}=\omega^{2} \tilde{S} \underline{\mathbf{d}}=0 \quad \text { and } \quad M_{\varepsilon} \tilde{S}^{T} D_{\tilde{V}}^{-1} \tilde{S} M_{\varepsilon} \underline{\mathbf{e}} \equiv 0
$$

we obtain the boundary value problem

$$
\begin{equation*}
\left(C^{T} M_{\nu} C+M_{\varepsilon} \tilde{S}^{T} D_{\tilde{V}}^{-1} \tilde{S} M_{\varepsilon}-\omega^{2} M_{\varepsilon}\right) \underline{\mathbf{e}}=0 \tag{26}
\end{equation*}
$$

where $D_{\tilde{V}}$ is the diagonal matrix of dual cell volumes $\tilde{V}\left(* \sigma^{0}\right)$. Taking into account the boundary conditions, Eq. (26) yields the form $A x=b$. Using independent set orderings, the permutations $P_{i}$ transform the matrix $A_{i}$ with $A_{0}=A$ into the form

$$
A_{i} \quad \longrightarrow \quad P_{i} A_{i} P_{i}^{T}=\left(\begin{array}{cc}
D_{i} & E_{i}^{T} \\
E_{i} & H_{i}
\end{array}\right)
$$

where $D_{i}$ is a diagonal, $E_{i}$, and $H_{i}$ are sparse matrices. We get the factorized system of linear equations

$$
\left(\begin{array}{cc}
I_{i} & 0  \tag{27}\\
E_{i} D_{i}^{-1} & I_{i}
\end{array}\right)\left(\begin{array}{cc}
D_{i} & E_{i}^{T} \\
0 & H_{i}-E_{i} D_{i}^{-1} E_{i}^{T}
\end{array}\right)\binom{y_{i, 1}}{y_{i, 2}}=\binom{c_{i, 1}}{c_{i, 2}}
$$

with $y_{i}=P_{i} x_{i}=\left(y_{i, 1}, y_{i, 2}\right)^{T}$ and $c_{i}=P_{i} b_{i}=\left(c_{i, 1}, c_{i, 2}\right)^{T}$. Using Krylov subspace methods, (27) can be solved iteratively (cf. [11, 12]).

## 4 Numerical results

We consider four academic examples to demonstrate the generality of the approach. The ability to optimize weights to improve the dual structure is very useful. Moving vertices of a primal mesh is potentially harmful, as it affects the surface shape. Therefore, only internal points are considered for optimization. For the four examples we compute the inverse of the matrix $M_{\varepsilon}$ to show the change of number of nonzero entries of $M_{\varepsilon}^{-1}$.
We use a stable iterative method for computing an approximate inverse of a square sparse matrix $A$ as follows:

$$
P_{n+1}=P_{n}\left(2 I-A P_{n}\right), \quad n=0,1,2, \ldots,
$$

under the condition $\left\|I-A P_{0}\right\|<1$. Then $P_{n} \rightarrow A^{-1}$ as $n \rightarrow \infty$.
The primal triangular mesh is generated using REGTET, a Fortran program for computing a regular tetrahedralization for a finite set of weighted points in 3d space (cf. [1, 2]). It is based on an algorithm by Edelsbrunner and Shah for constructing regular tetrahedralizations with incremental topological flipping (cf. [6]).

Example 1. The first example has the form of a crystal (cf. Fig. 3). The colored areas represent different material parameters. We define a rectangular regular grid on the surface of a rectangular polyhedron that contains the set of input points $\left\{\mathrm{x}_{1}, \ldots, \mathrm{x}_{8}\right\}$ to become, together with this set of input points, the set for which a tetrahedralization is to be computed. For $n_{\text {add }} \geq 2$ for each facet of the polyhedron a set of $n_{\text {add }} \times n_{\text {add }}$ points is generated. This set defines a rectangular regular grid and contains the four vertices of the facet. The union of the six sets thus generated define the rectangular grid on the surface of the polyhedron with $n_{p o l}$ points:

$$
n_{\text {pol }}=6\left(n_{\text {add }}-2\right)^{2}+12\left(n_{\text {add }}-2\right)+8=6 n_{\text {add }}^{2}-12 n_{\text {add }}+8 .
$$

In Table 2 \#tet denotes the number of all tetrahedra and \#sctet the number of self-centered tetrahedra. The weights of the input points and the weights of the points on the surface of the rectangular polyhedron are $w_{i}=0.00$. The finished weights for $n_{\text {add }}=0$ at the end of the iteration are given in Fig. 3. This set of weights is not unique. However the number of selfcentered tetrahedra has increased significantly.

Table 2: The number of self-centered tetrahedra for $\star^{3}-\mathrm{HOT}_{2,2}$ (Example 1).

| $n_{\text {add }}$ | $(\mathcal{T}, \mathcal{D})$ |  |  | $(\mathcal{R T}, \mathcal{P D})$ at first |  |  | $(\mathcal{R T}, \mathcal{P D})$ finished |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | \#tet | \#sctet | \% | \#tet | \#sctet | \% | \#tet | \#sctet | \% |
| 0 | 12 | 0 | 0.00 | 12 | 0 | 0.00 | 12 | 10 | 83.33 |
| 2 | 48 | 0 | 0.00 | 48 | 0 | 0.00 | 47 | 20 | 42.55 |
| 3 | 95 | 14 | 14.74 | 95 | 14 | 14.74 | 83 | 59 | 71.08 |
| 4 | 170 | 50 | 29.41 | 170 | 50 | 29.41 | 165 | 116 | 70.30 |
| 5 | 277 | 48 | 17.33 | 277 | 48 | 17.33 | 269 | 166 | 61.71 |

In Table 3, the dimension $n_{e}$ and the number of nonzero entries of the matrices $M_{\varepsilon}$ and $M_{\varepsilon}^{-1}$ are shown. While the weights of the input points in Table 4 are also $w_{i}=0.00$, the weights

$\begin{aligned} & \mathrm{x}_{\mathbf{1}}=\left(\begin{array}{lll}0.0, & 0.0, & 0.0\end{array}\right) \\ & \mathrm{x}_{\mathbf{2}}=\left(\begin{array}{lll}-1.0, & 0.0, & 0.0\end{array}\right) \\ & \mathrm{x}_{3}=\left(\begin{array}{lll}1.0, & 0.0, & 0.0\end{array}\right) \\ & \mathrm{x}_{4}\end{aligned}=\left(\begin{array}{lll}0.0, & -1.0, & 0.0\end{array}\right)$,

|  | $w_{i}$ at first | $w_{i}$ finished |
| :--- | ---: | ---: |
| $\mathbf{1}$ | 0.00 | -0.005075 |
| 2 | 0.00 | 0.477244 |
| 3 | 0.00 | 0.716525 |
| $\mathbf{4}$ | 0.00 | 0.477620 |
| 5 | 0.00 | 0.729235 |
| 6 | 0.00 | 0.746571 |
| 7 | 0.00 | 1.859071 |
| $\mathbf{8}$ | 0.00 | 0.065864 |

Figure 3: The crystal.

Table 3: The number of nonzero entries of $M_{\varepsilon}$ and $M_{\varepsilon}^{-1}$ (Example 1).

| $n_{\text {add }} \\|$ |  | $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ at first |  |  | $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ finished |  |
| :---: | ---: | ---: | ---: | ---: | ---: | ---: |
|  | $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ | $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ |
| 0 | 23 | 167 | 529 | 23 | 67 | 83 |
| 2 | 69 | 673 | 4761 | 68 | 484 | 2480 |
| 3 | 152 | 1176 | 21908 | 139 | 511 | 4561 |
| 4 | 287 | 2135 | 76739 | 282 | 1124 | 23640 |
| 5 | 478 | 3560 | 228484 | 470 | 2020 | 75474 |

Table 4: The number of self-centered tetrahedra for $\star^{3}-\mathrm{HOT}_{2,2}$ in dependence of the weights on the surface points (Example 1).

| $n_{\text {add }}$ |  |  |  |  |  |  |  |
| :---: | :---: | ---: | ---: | ---: | ---: | ---: | ---: |
|  | $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ at first |  |  | $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ finished |  |  |  |
|  | \#tet | \#sctet | $\%$ | \#tet | \#sctet | $\%$ |  |
| 2 | 48 | 0 | 0.00 | 47 | 20 | 42.55 |  |
| 3 | 99 | 15 | 15.15 | 92 | 58 | 63.04 |  |
| 4 | 167 | 46 | 27.54 | 164 | 115 | 70.12 |  |
| 5 | 284 | 9 | 3.17 | 261 | 144 | 55.17 |  |

on the surface are $w_{i}=1.00$. The iterative behavior between $w_{i}=0.00$ and $w_{i}=1.00$ on the surface of the polyhedron is different. This example has no internal points for vertex position optimization.

Example 2. The second example is a rectangular bar that is crossed by another bar (cf. Fig. 4). As in the first example, here too the colored areas represent different material parameters. In


Figure 4: A rectangular bar that is crossed by anaother rectangular bar.
Table 5, the numbers of self-centered tetrahedra are shown both in dependence of the weights of the input points and vertex/weight optimization. The weights of the input points are changed as a function of the terms

$$
\begin{array}{lll} 
& i(\bmod 8) \cdot 0.10, & (\bar{w}) \\
& i(\bmod 8) \cdot 0.12, & (\tilde{w}) \\
\text { and } & i(\bmod 9) \cdot 0.08, & (\hat{w})
\end{array}
$$

respectively. Also in this example, the iterative behavior is different in dependence of the weights of the input points.

Table 5: The number of self-centered tetrahedra for $\star^{3}-\mathrm{HOT}_{2,2}$ both in dependence of the weights of the input points and vertex/weight optimization (Example 2).

| $(\mathcal{R T}, \mathcal{P D})$ at first |  |  | $(\mathcal{R T}, \mathcal{P D})$ finished (weight optim.) |  |  | $(\mathcal{R T}, \mathcal{P D})$ finished (vertex/weight optim.) |  |  | $w_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| \#tet | \#sctet | \% | \#tet | \#sctet | \% | \#tet | \#sctet | \% |  |
| 44 | 4 | 2.78 | 141 | 112 | 79.43 | 143 | 109 | 76.22 | 0 |
| 141 | 48 | 34.04 | 141 | 106 | 75.18 | 141 | 99 | 70.21 | $\bar{w}$ |
| 141 | 49 | 34.75 | 135 | 101 | 74.81 | 138 | 97 | 70.29 | $\tilde{w}$ |
| 144 | 36 | 25.00 | 142 | 102 | 71.83 | 144 | 113 | 78.47 | $\hat{w}$ |

In Table 6, the number of nonzero entries of the matrices $M_{\nu}, M_{\varepsilon}$, and $M_{\varepsilon}^{-1}$ are shown. The values $n_{e}$ and $n_{f}$ are the dimensions of the material matrices $M_{\varepsilon}$ and $M_{\nu}$, respectively. In Fig. 5 this matrices are shown with no weights of input points. The term $n_{n z}$ represents the number of nonzero elements of $M_{\varepsilon}$ and $M_{\nu}$, respectively. Except for the initialization $w_{i} \leftarrow \hat{w}$, the weight optimization yields better results than the vertex position/weight optimization.

Table 6: The number of nonzero entries of $M_{\nu}, M_{\varepsilon}$, and $M_{\varepsilon}^{-1}$ (Example 2).

| $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ at first |  |  | $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ finished (weight optim.) |  |  | ( $\mathcal{R} \mathcal{T}, \mathcal{P D}$ ) finished (vertex/weight optim.) |  |  | $w_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ | $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ | $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ |  |
| 255 | 1829 | 65025 | 250 | 648 | 5242 | 254 | 716 | 13238 | 0 |
| 252 | 1210 | 60032 | 250 | 654 | 14056 | 252 | 838 | 14534 | $\bar{w}$ |
| 252 | 1214 | 57612 | 242 | 646 | 13814 | 249 | 851 | 12539 | $\tilde{w}$ |
| 255 | 1415 | 62007 | 253 | 709 | 13017 | 255 | 757 | 8367 | $\hat{w}$ |
| $n_{f}$ | $M_{\mu}$ |  | $n_{f}$ | $M_{\mu}$ |  | $n_{f}$ | $M_{\mu}$ |  |  |
| 340 | 1834 |  | 333 | 637 |  | 338 | 710 |  | 0 |
| 334 | 1352 |  | 333 | 703 |  | 334 | 800 |  | $\bar{w}$ |
| 334 | 1336 |  | 320 | 690 |  | 328 | 792 |  | $\tilde{w}$ |
| 340 | 1510 |  | 336 | 772 |  | 340 | 686 |  | $\hat{w}$ |

Example 3. The third example is a grid of points over the interior of a cube in 3d space with edge lengths $[1,5] \times[1,6] \times[1,7]$. In each coordinate direction, the grid uses 5 points. These points are equally spaced. Thus, the number of vertices equals 125 . In Table 7 , the numbers of self-centered tetrahedra are shown both in dependence of the weights of the input points and vertex/weight optimization. In Table 8, the number of nonzero entries of the matrices $M_{\nu}, M_{\varepsilon}$, and $M_{\varepsilon}^{-1}$ are shown.


Figure 5: The nonzero pattern of matrices $M_{\varepsilon}$ and $M_{\nu}$.

Example 4. The fourth example is a grid of points over the interior of a tetrahedron in 3d. The grid is defined by specifying the coordinates of an enclosing tetrahedron. The coordinates are $(0,0,0),(10,0,0),(0,10,0)$, and $(0,0,10)$. Each edge of the tetrahedron is devided in 5 subintervals. Thus, the number of vertices equals 56 . In Table 9 , the numbers of self-centered tetrahedra are shown both in dependence of the weights of the input points and vertex/weight optimization. In Table 10, the number of nonzero entries of the matrices $M_{\nu}, M_{\varepsilon}$, and $M_{\varepsilon}^{-1}$ are shown.

Table 7: The number of self-centered tetrahedra for $\star^{3}-\mathrm{HOT}_{2,2}$ both in dependence of the weights of the input points and vertex/weight optimization (Example 3).

| $(\mathcal{R T}, \mathcal{P D})$ at first |  |  | ( $\mathcal{R} \mathcal{T}, \mathcal{P D}$ ) finished (weight optim.) |  |  | ( $\mathcal{R} \mathcal{T}, \mathcal{P D}$ ) finished (vertex/weight optim.) |  |  | $w_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| \#tet | \#sctet | \% | \#tet | \#sctet | \% | \#tet | \#sctet | \% |  |
| 38 | 0 | 0.00 | 370 | 313 | 84.59 | 59 | 308 | 85.79 | 0 |
| 384 | 87 | 22.66 | 365 | 275 | 75.34 | 361 | 317 | 87.81 | $\bar{w}$ |
| 384 | 88 | 22.92 | 366 | 247 | 67.49 | 319 | 208 | 65.20 | $\tilde{w}$ |
| 384 | 93 | 24.22 | 369 | 284 | 76.96 | 372 | 287 | 77.15 | $\hat{w}$ |

Table 8: The number of nonzero entries of $M_{\nu}, M_{\varepsilon}$, and $M_{\varepsilon}^{-1}$ (Example 3).

| $(\mathcal{R T}, \mathcal{P D})$ at first |  |  | $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ finished (weight optim.) |  |  | $(\mathcal{R T}, \mathcal{P D})$ finished (vertex/weight optim.) |  |  | $w_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ | $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ | $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ |  |
| 604 | 4850 | 364816 | 586 | 1286 | 24110 | 579 | 1599 | 15211 | 0 |
| 604 | 3954 | 349294 | 581 | 1737 | 48399 | 577 | 1467 | 15325 | $\bar{w}$ |
| 604 | 3990 | 344586 | 582 | 2092 | 115872 | 515 | 2411 | 90057 | $\tilde{w}$ |
| 604 | 3666 | 346936 | 587 | 1609 | 42553 | 591 | 2231 | 80457 | $\hat{w}$ |
| $n_{f}$ | $M_{\mu}$ |  | $n_{f}$ | $M_{\mu}$ |  | $n_{f}$ | $M_{\mu}$ |  |  |
| 864 | 4958 |  | 834 | 1432 |  | 814 | 1408 |  | 0 |
| 864 | 4082 |  | 824 | 1822 |  | 816 | 1340 |  | $\bar{w}$ |
| 864 | 4062 |  | 826 | 2126 |  | 725 | 2025 |  | $\tilde{w}$ |
| 864 | 3998 |  | 833 | 1741 |  | 840 | 1850 |  | $\hat{w}$ |

Table 9: The number of self-centered tetrahedra for $\star^{3}-\mathrm{HOT}_{2,2}$ both in dependence of the weights of the input points and vertex/weight optimization (Example 4).

| $(\mathcal{R T}, \mathcal{P D})$ at first |  |  | $(\mathcal{R T}, \mathcal{P D})$ finished (weight optim.) |  |  | $(\mathcal{R T}, \mathcal{P D})$ finished (vertex/weight optim.) |  |  | $w_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| \#tet | \#sctet | \% | \#tet | \#sctet | \% | \#tet | \#sctet | \% |  |
| 124 | 1 | 0.81 | 118 | 77 | 65.25 | 118 | 83 | 70.34 | 0 |
| 122 | 35 | 28.69 | 115 | 76 | 66.09 | 115 | 80 | 69.57 | $\bar{w}$ |
| 122 | 35 | 28.69 | 115 | 77 | 66.96 | 109 | 77 | 70.64 | $\tilde{w}$ |
| 120 | 42 | 35.00 | 112 | 97 | 86.61 | 118 | 92 | 77.97 | $\hat{w}$ |

## 5 Conclusions

A combination of a mainly orthogonal and locally barycentric mesh is used to discretize the Maxwell's equations in integral form using FIT. The constitutive relations are discretized using

Table 10: The number of nonzero entries of $M_{\nu}, M_{\varepsilon}$, and $M_{\varepsilon}^{-1}$ (Example 4).

| $(\mathcal{R T}, \mathcal{P D})$ at first |  |  | $(\mathcal{R} \mathcal{T}, \mathcal{P D})$ finished (weight optim.) |  |  | $(\mathcal{R T}, \mathcal{P D})$ finished (vertex/weight optim.) |  |  | $w_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ | $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ | $n_{e}$ | $M_{\varepsilon}$ | $M_{\varepsilon}^{-1}$ |  |
| 229 | 1609 | 52441 | 217 | 777 | 18149 | 219 | 821 | 14499 | 0 |
| 227 | 1167 | 45413 | 214 | 734 | 12358 | 214 | 750 | 9486 | $\bar{w}$ |
| 227 | 1167 | 45413 | 214 | 716 | 12314 | 206 | 698 | 5072 | $\tilde{w}$ |
| 225 | 1029 | 44535 | 213 | 433 | 1391 | 223 | 645 | 6657 | $\hat{w}$ |
| $n_{f}$ | $M_{\mu}$ |  | $n_{f}$ | $M_{\mu}$ |  | $n_{f}$ | $M_{\mu}$ |  |  |
| 298 | 1640 |  | 283 | 733 |  | 284 | 688 |  | 0 |
| 294 | 1276 |  | 277 | 715 |  | 277 | 681 |  | $\bar{w}$ |
| 294 | 1276 |  | 277 | 693 |  | 264 | 624 |  | $\tilde{w}$ |
| 290 | 1170 |  | 272 | 432 |  | 286 | 578 |  | $\hat{w}$ |

the Hodge star operator. It relates differential forms of different degrees. The duality between regular triangulations and power diagrams allows a different choice on the dual mesh once the primal mesh is fixed. For each tetrahedron that is not self-centered we construct the constitutive matrices by using the microcell method. The Hodge-optimized triangulation strategy makes more self-centered tetrahedra and thus improved one or more of the discrete Hodge stars. Due to efficiency reasons the set of weights and vertices/weights, respectively is a non-optimal minimum. However, using the weight optimization, the number of non-zero elements of the material matrices is important reduced. The vertex position optimization alone hardly improved the dual meshes. An open problem is the construction of the inverse of the material matrix $M_{\varepsilon}$.

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[^0]:    2010 Mathematics Subject Classification. 35Q61, 65F10, 65F15, 65N22, 65N50.
    Key words and phrases. Optimal triangulations, discrete Hodge star, Maxwell's equations, finite integration technique, microcell method, linear algebraic equations.

