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Beam propagation in geometries with piece-wise constant refractive index.

It is well known that components of electric and magnetic fields satisfy "continuity" conditions at material interfaces. Here we explore the less known conditions that are obeyed by *derivatives* of these fields.

From the simulation or numerical point of view, an interface prevents us from using the same stencil as in the bulk material, so we can not obtain approximations of spatial derivatives which appear in propagation equations the same way. The problem therefore is how to tailor solutions on each side of an interface into a single global function that correctly reflects properties of Maxwell fields across a material boundary. One method to deal with this takes advantage of interface conditions for the field derivatives. There is in fact a whole hierarchy of derivative relations, and these can serve as basis to construct simulation schemes for finite-difference Maxwell solvers. Here we restrict ourselves to the lowest order derivative conditions, and show how they can be applied in the BPM context. This material applies to waveguiding structures with piece-wise constant material properties.

15.1 Boundary conditions for field derivatives in Maxwell's equations

Assume a sharp interface between two homogeneous, non-magnetic dielectrics. Let us orient our local coordinate system such that the interface coincides with $x = 0$ plane. The textbook boundary conditions for fields then require that fields

$$D_x \quad E_y \quad E_z \tag{15.1}$$

are continuous across the interface (at least when no surface charges are present), as are all components of the magnetic field (when no surface currents exists).

The question is what are the interface conditions for the first (and higher) spatial derivatives of the electromagnetic fields? Also, is it possible to incorporate such conditions into beam propagation simulation methods?

The boundary conditions in question can be derived in a systematic way. The interested reader is referred to Ref. XXX which show this in a straightforward, but little abstract manner. Here we pursue a perhaps more concrete approach.

Take these two Maxwell equations first:

$$\nabla \times \boldsymbol{H} = \partial_t \boldsymbol{D} \quad \nabla . \boldsymbol{H} = 0 \ , \tag{15.2}$$

and write them in an explicit, component-by-component form,

$$
\begin{aligned}
0 &= \partial_x H_x + \partial_y H_y + \partial_z H_z \\
\partial_t D_x &= \partial_y H_z - \partial_z H_y \\
\partial_t D_y &= \partial_z H_x - \partial_x H_z \\
\partial_t D_z &= \partial_x H_y - \partial_y H_x \ .
\end{aligned} \tag{15.3}
$$

Obviously, these component equations are invalid right at the interface ($x = 0$) since the derivatives in general do not exist there (keep in mind that we are considering an ideal, infinitely sharp boundary between two materials). However, we can subtract two sets of equations between two infinitely close points, each on one side, and inspect the resulting terms that remain after elimination of quantities that we know must be continuous.

We use ΔQ to denote the jump in the quantity Q, i.e. $\Delta Q \equiv Q(x = 0^+) - Q(x = 0^-)$. After application of the standard continuity conditions to obtain

$$
\begin{aligned}
0 &= +\Delta \partial_x H_x \\
0 &= 0 \\
\Delta\epsilon \partial_t E_y &= -\Delta \partial_x H_z \\
\Delta\epsilon \partial_t E_z &= +\Delta \partial_x H_y
\end{aligned} \tag{15.4}
$$

From here we see that normal derivatives of parallel magnetic fields suffer a jump across the interface. Thus, while they are continuous functions in space, material boundary still manifests itself although in a subtle manner, namely as a cusp.

However, since we have formulated our propagation equation in the language of electric fields, let us repeat the same procedure for the second set of Maxwell equations, namely

$$
\nabla \times \boldsymbol{E} = -\partial_t \boldsymbol{B} \quad \nabla . \boldsymbol{D} = 0 \tag{15.5}
$$

$$
\begin{aligned}
0 &= \partial_x D_x + \partial_y D_y + \partial_z D_z \\
-\partial_t B_x &= \partial_y E_z - \partial_z E_y \\
-\partial_t B_y &= \partial_z E_x - \partial_x E_z \\
-\partial_t B_z &= \partial_x E_y - \partial_y E_x \ .
\end{aligned} \tag{15.6}
$$

Apply the jump operator Δ, and commute it with quantities and derivatives which are continuous across the boundary to obtain:

$$
\begin{aligned}
0 &= \Delta \partial_x D_x + (\partial_y E_y + \partial_z E_z)\Delta\epsilon \\
0 &= 0 \\
0 &= \partial_z D_x \Delta(1/\epsilon) - \Delta \partial_x E_z \\
0 &= \Delta \partial_x E_y - \partial_y D_x \Delta(1/\epsilon) \ .
\end{aligned} \tag{15.7}
$$

Above, we have also eliminated field E_x which is discontinuous in favor of D_x, so that derivative jumps can be all expressed in terms of fields which have a defined value at the interface:

$$
\begin{aligned}
\Delta \partial_x D_x &= -\Delta(\epsilon)(\partial_y E_y + \partial_z E_z) \\
\Delta \partial_x E_y &= +\Delta(1/\epsilon)\partial_y D_x \\
\Delta \partial_x E_z &= +\Delta(1/\epsilon)\partial_z D_x
\end{aligned} \tag{15.8}
$$

These constraints suggest a numerical wave-propagation method for structures with piece-wise constant material properties. We can use homogeneous-medium discretization for grid-regions that are contained within a constant-index regions. The interface conditions then can be used to obtain electric field samples located directly at the material boundaries, and result in coupling between constant-index regions.

In the BPM context, it is also possible to eliminate the longitudinal electric component. Again, one can take advantage of the piece-wise constant index assumption, which means that not only $\nabla.D = 0$ but also $\nabla.E = 0$ everywhere where the derivatives needed to form divergences are properly defined, i.e. away from interfaces, but also arbitrarily close to them.

Thus, we can write

$$\nabla.\boldsymbol{D} = \epsilon(\partial_x E_x + \partial_y E_y + \partial_z E_z) = 0 \tag{15.9}$$

arbitrarily close to a sharp material interface. The constant permittivity has been pulled out of the derivative terms, because it is a piece-wise constant function. This in turn implies that

$$\partial_x E_x + \partial_y E_y + \partial_z E_z = 0 \ , \tag{15.10}$$

and application of the jump operator to this yields

$$\Delta \partial_x E_x = 0 \ . \tag{15.11}$$

In other words, normal derivative of the normal component of the electric field is continuous at the sharp interface. This makes it possible to reduce the system of equations needed for BPM, so that only transverse field components must be propagated,

$$\begin{aligned} \Delta \partial_x E_x &= 0 \\ \Delta \partial_x E_y &= +\Delta(1/\epsilon)\partial_y D_x \ . \end{aligned} \tag{15.12}$$

The minor complication is that the both the electric intensity and electric induction enter these relations and will therefore appear in the discretized equations. However, one can always locally switch from one field to the other, depending on what value is needed. One practical way to deal with this is to store for grid nodes located at material boundaries those components of the field that are continuous. The corresponding normal and parallel polarization components then can be evaluated based on the local orientation of the interface.

15.2 Interface derivative matching method

For simplicity, let us consider a situation in which the material boundary runs along one of the numerical grid axes.

15.2.1 Normal field components

The natural variable to consider in the vicinity of interface is one that is continuous across such a boundary. In the case of the normal component, this is of course the electric induction D_x.

Consider a grid node located at the interface, and denote D_L, D_C, and D_R values at grid-nodes which are left, at, and right of the interface. To keep notation simple, also assume that the grid spacing Δx is the same on both sides. Then the condition that requires continuity of the normal derivative of the electric field

$$\Delta \partial_x E_x = 0$$

can be approximated by (x-components are assumed in these expressions):

$$\frac{1}{\epsilon_L}\frac{D_C - D_L}{\Delta x} = \frac{1}{\epsilon_L}\frac{D_R - D_C}{\Delta x} \ , \tag{15.13}$$

where the electric field has been expressed in terms of the continuous displacement field. From here, we have

$$D_C = \frac{\epsilon_L \epsilon_R}{\epsilon_L + \epsilon_R}(E_L + E_R) \ . \tag{15.14}$$

This is the field value that, to second order accuracy in Δx, ensures that the one-sided derivatives of electric intensity are equal (while the field intensity itself is discontinuous).

Thus, when the numerical algorithm needs e.g. $\partial_{xx} E_x$ at a point next to the interface, one can write

$$\begin{aligned} E_C^+ &= \frac{\epsilon_L}{\epsilon_L + \epsilon_R}(E_L + E_R) \\ E_C^- &= \frac{\epsilon_R}{\epsilon_L + \epsilon_R}(E_L + E_R) \end{aligned} \tag{15.15}$$

for values at the interface when approaching from a defined direction. This is then sufficient to approximate spatial derivatives in the immediate vicinity of the boundary. For example, to approximate discrete Laplacian values,

$$\begin{aligned} (\partial_{xx} E_x)_R &\approx (E_C^+ - 2E_R + E_{RR})/\Delta x^2 \\ (\partial_{xx} E_x)_L &\approx (E_{LL} - 2E_L + E_C^-)/\Delta x^2 \ , \end{aligned} \tag{15.16}$$

with double-subscripts indicating the points that are next-nearest neighbors of the node located at the interface. The effect is that the discretization schemes on different sides of the boundary are coupled.

15.2.2 Parallel polarization components

This time we are going to use the second interface condition, namely

$$\Delta \partial_x E_y = +\Delta(1/\epsilon)\partial_y D_x = \frac{\epsilon_L - \epsilon_R}{\epsilon_R \epsilon_L}\partial_y D_x \tag{15.17}$$

One can approximate right hand side by a finite difference along the boundary between the two materials (which the y direction in the present case). For example:

$$(\partial_y D_x)_C = \frac{1}{2\Delta y}(D_C(y + \Delta y) - (D_C(y - \Delta y) \ , \tag{15.18}$$

and a three-point, one-sided finite differences can be applied close to interface corners (so as to preserve the same accuracy order). Note that this means that the interface values of the normal component of electric induction must be stored. The relevant boundary constraint requires

$$\Delta \partial_x E_y = \frac{\epsilon_L - \epsilon_R}{\epsilon_R \epsilon_L}(\partial_y D_x)_C \tag{15.19}$$

where the right-hand-side is assumed to be discretized in the form shown above. Next, one must set the $E_y = E_C$ value located at the interface such that the above condition is fulfilled, which leads to

$$\frac{E_R - E_C}{\Delta x} - \frac{E_C - E_L}{\Delta x} = \frac{\epsilon_L - \epsilon_R}{\epsilon_R \epsilon_L}(\partial_y D_x)_C \quad \text{or} \quad E_C = \frac{E_L + E_R}{2} - \Delta x \frac{\epsilon_L - \epsilon_R}{\epsilon_R \epsilon_L}(\partial_y D_x)_C \tag{15.20}$$

Note that the expression for the right hand side also contains Δy so it does not vanish in the continuum limit $\Delta x, y \to 0$. Having calculated the interface value of E_y in this way, it can be used in evaluation of Laplacian expressions on both sides of the interface. The scheme couples field samples at both sides of the interface, and also values of the continuous component along the interface.

In practical terms, it requires modification of discretized equation at all point adjacent to the material boundary. The implementation is relatively simple for geometries in which all interfaces are parallel to one of the grid axes, which is in fact frequently the case. The resulting modified discretization scheme can be applied equally to finite-difference (in z) schemes and to the method of lines.