Publication I


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Performance of convolutional PML absorbing boundary conditions in finite-difference time-domain SAR calculations

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Received 13 August 2007, in final form 22 October 2007
Published 19 November 2007
Online at stacks.iop.org/PMB/52/7183

Abstract
The performance of perfectly matched layer (PML) absorbing boundary conditions is studied for finite-difference time-domain (FDTD) specific absorption rate (SAR) assessment, using convolutional PML (CPML) implementation of PML. This is done by investigating the variation of SAR values when the amount of free-space layers between the studied object and PML boundary is varied. Plane-wave exposures of spherical and rectangular objects and a realistic human body model are considered for testing the performance. Also, some results for dipole excitation are included. Results show that no additional free-space layers are needed between the numerical phantom and properly implemented CPML absorbing boundary, and that the numerical uncertainties due to CPML can be made negligibly small.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The finite-difference time-domain method (Taflove and Hagness 2005) is the most popular method for the assessment of human SAR values under exposure to radio-frequency electromagnetic fields. In such SAR calculations, it is usually required to position the models in free space, which is implemented using absorbing boundary conditions (ABCs). The most popular choice is the perfectly matched layer (PML) (Bérenger 1994) based ABC. The performance and implementation of PML play a major role in the memory requirements of large problems, as nonefficient PML may require additional free-space layers between the object and the PML.

Several recent papers have discussed the applicability of PML absorbing boundary conditions in FDTD SAR calculations. It was reported in Wang et al (2006) that uniaxial PML (UPML) (Sacks et al 1995) absorbing boundary conditions may cause significant error in whole-body SAR values in a homogeneous muscle sphere. It was concluded that a thick
free-space region between the numerical phantom and the UPML boundaries is required for accurate whole-body SAR results. In Findlay and Dimbylow (2006), the NORMAN phantom and split-field PML were studied. The results showed little variation in the whole-body-averaged SAR values when the distance between the voxel phantom and PML-ABC was varied. Also, increasing the PML width above six cells had a little effect on the SAR values.

In this work, convolutional PML (CPML) (Roden and Gedney 2000) absorbing boundary conditions are employed for SAR calculation. The objective is to verify the performance of CPML and also find good CPML parameters for SAR calculation.

2. Convolutional PML

CPML (Roden and Gedney 2000) is an efficient implementation of PML when the coordinate stretching variables \( s_u \) (Chew and Weedon 1994) are of the complex-frequency shifted (CFS) form Kuzuoglu and Mittra (1996), i.e.

\[
 s_u = k + \frac{\sigma}{\alpha + j\omega \epsilon_0}, \quad u \in \{x, y, z\}. \tag{1}
\]

In what is to follow, the PML will be called regular PML when \( \alpha = 0 \), and CFS-PML when \( \alpha > 0 \). In addition to CPML, there are several other implementations of regular PML, which include the original split-field PML (Bérenger 1994) and uniaxial PML (UPML) (Sacks et al. 1995), which are used in FDTD SAR calculations perhaps more commonly than the CPML. The performances of the UPML and split-field PML are almost identical, while the performance of the corresponding regular PML implemented with CPML might be slightly better in practice (Bérenger 2002). Both the regular PML and CFS-PML have their limitations: the regular PML is inefficient in absorbing evanescent waves (Bérenger 1999), while in turn, CFS-PML may have problems with the absorption of propagating waves, because \( \alpha > 0 \) (Bérenger 2002, Correia and Jin 2006).

In a continuous space, PML is able to absorb incident waves perfectly, but spurious numerical reflections occur in a discretized FDTD space. These reflections can be reduced by grading the coordinate stretching variables inside the PML. In this work, polynomial grading, as shown in figure 1, is used. Based on a large number of test simulations using a small muscle sphere as in section 4.1, the following values for the parameters in figure 1 proved to
Figure 2. The CPML test setup. The distance from the object to the CPML boundary is $d$.

be effective for the CFS-PML:

$$\sigma_{\text{max}} = \sigma_{\text{opt}}(m, \Delta) = \frac{0.8(m + 1)}{\eta/\Delta},$$

as in (Taflove and Hagness 2005), where $\Delta$ is the resolution of the FDTD discretization and $\eta \approx 377 \Omega$. The other parameters in the figure were $\kappa_{\text{max}} = 5$, $\alpha_{\text{max}} = 0.05$, $m = 3$ and $m_\alpha = 1$. For comparison, also the regular PML was studied, for which the parameters were the same as in the CFS-PML, except $\kappa_{\text{max}} = 1$ and $\alpha_{\text{max}} = 0$. Generally, the optimal choice of the parameters depends on the geometry, resolution and frequency range of the problem.

Parameter $\alpha$ in (1) governs the absorption of evanescent fields. Typically, $\alpha$ should be larger for problems with strongly evanescent waves, and smaller for problems with only weakly evanescent fields. The optimal value for parameter $\alpha$ is approximately independent of the frequency, being inversely proportional to the size of the problem (Bérenger 2002). In this work, a linear scaling of $\alpha$ was used, which is thought to combine the benefits of constant-$\alpha$ CFS-PML and regular PML (Taflove and Hagness 2005): larger $\alpha$ near the air–PML boundary allows evanescent waves to penetrate into the PML without reflection, and smaller $\alpha$ near the outer boundary of PML improves the absorption of propagating waves.

3. Methods

The performance of the absorbing boundary is investigated by using an approach similar to Wang et al (2006) and Findlay and Dimbylow (2006), i.e. an object is positioned in free space surrounded by PML boundaries. The setup is illustrated in figure 2. The object is exposed to a linearly polarized plane wave, which is implemented using the total-field/scattered-field technique and sinusoidal excitation. The distance $d$ from the object to PML is varied, and SAR inside the object is calculated for each distance.

The results are presented as figures that plot the distance $d$ versus the variation of whole-body SAR values. The variation is calculated relative to the case where the distance $d$ is large and the PML is thick. If the ABC was ideal, the scattered field would be absorbed perfectly regardless of the distance, and there would be no variation of SAR values. Thus, the smaller the variation of SAR with the distance $d$, the better the performance of PML. This procedure
Table 1. Material parameters of 2/3 muscle.

<table>
<thead>
<tr>
<th>Frequency</th>
<th>$\sigma$ (S m$^{-1}$)</th>
<th>$\epsilon_r$</th>
<th>$\rho$ (kg m$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 MHz</td>
<td>0.48</td>
<td>46.0</td>
<td>1000</td>
</tr>
<tr>
<td>1 GHz</td>
<td>0.65</td>
<td>36.5</td>
<td>1000</td>
</tr>
<tr>
<td>2 GHz</td>
<td>1.00</td>
<td>37.3</td>
<td>1000</td>
</tr>
<tr>
<td>5 GHz</td>
<td>2.78</td>
<td>34.7</td>
<td>1000</td>
</tr>
</tbody>
</table>

is employed to study the performance of PML in three test cases, which represent different geometries and problem sizes.

The first test case is a small homogeneous 2/3-muscle sphere, whose radius is 2.5 cm, and which is constructed using staircase approximation. The material parameters of 2/3 muscle can be found in table 1. The sphere is exposed either to a plane wave or a short dipole which is positioned 2 cm from the surface of the sphere. The direction of the dipole is perpendicular to the sphere radial direction. The results include comparing the performance of CFS-PML with regular PML, and the influence of PML thickness. Simulations are conducted at various frequencies from 100 MHz to 5 GHz.

The second test case is a homogeneous 2/3-muscle box phantom, whose dimensions are 6 cm $\times$ 12 cm $\times$ 12 cm. The propagating direction of the incident plane wave is parallel to the short axis of the box. The dependence of the PML performance on the frequency and FDTD resolution are studied. Additionally, some effects of tuning the CPML parameters in figure 1 are presented.

The third test case is a realistic human body model, NORMAN (Dimbylow 1997), which is exposed to a plane wave. The incident plane wave is vertically polarized and propagating towards the face of the phantom. The material parameters of tissues are based on Gabriel et al (1996a, 1996b, 1996c). Both whole-body and localized 10 g-averaged SAR are considered. The 10 g-averaged SAR is determined using the guidelines in IEEE (2002, C95.3-2002, annex E). The simulations for NORMAN are conducted at frequencies 300 MHz and 2.14 GHz.

4. Results

4.1. Small muscle sphere

Figure 3 shows the variation of whole-body-averaged SAR in the sphere under plane-wave exposure as a function of the PML–sphere distance for CFS and regular PMLs for two PML thicknesses $D$ at the investigated frequencies.

Figures 3(a) and (b) show the plane-wave results for frequencies 100 MHz and 1 GHz. It can be clearly seen that placing regular PML too close to the sphere may cause error in SAR values. This error is due to the incapability of regular PML to absorb evanescent waves of the scattered field, the magnitude of which decays exponentially. Increasing the width of the PML reduces this error only a little. Also, it can be seen that the error caused by low-performance PML may cause both over- and underestimation in the evaluation of the whole-body SAR. When CFS-PML is used, there is no additional error due to the small sphere–PML distance. That means, the evanescent fields are absorbed well by the PML. The variation of SAR values seems to be somewhat sinusoidal in the 1 GHz case, and increasing the width of the PML by just one layer reduces the error significantly.

In the 2 GHz and 5 GHz cases in figures 3(c) and (d), regular PML performs better than in the lower frequency cases, so the differences compared to CFS-PML are somewhat smaller.
The best frequency for the regular PML seems to be 2 GHz, where it actually outperforms the CFS-PML by a slim margin. Similarly to the 1 GHz case, the variation of SAR for CFS-PML is 'sinusoidal'. Even though the variation for regular PML might be slightly smaller, it does not follow such a clear pattern, which might again be due to nonperfect absorption of evanescent fields near the sphere. At 5 GHz, the CFS-PML is clearly more efficient than the regular PML. Compared to the plane-wave-exposed sphere results in Wang et al. (2006), the errors presented here are much smaller, even in the regular-PML case. In that paper, e.g. a 10 cm-radius sphere at 460 MHz gave almost 10% variation with a 12-cell thick UPML. In the present results, the approximately corresponding case—a 2.5 cm sphere at 2000 MHz—gives a little over 1% variation with 4-cell thick CPML, and a very small variation for 5-cell CPML. Here, in the case of regular PML at 1 GHz and 100 MHz, the error is significant only at small CPML–sphere distances, and quickly decreases for larger distances. However, in Wang et al (2006), the variation of SAR remains significantly larger for relatively large distances.

The above simulations were repeated when the plane-wave excitation was replaced by a short electrical dipole. The results are shown in figure 4, and they appear to be quite similar to the plane-wave case. Again, CFS-PML seems to perform equally well for all frequencies, and regular PML appears to have problems at the lower frequencies.

It is quite obvious from the results that, when the CPML parameters are chosen correctly, such as in the employed CFS-PML, the error caused by the ABC is very small for a wide frequency range. The CFS-PML functioned approximately equally well for all frequencies,

### Table: Variation in SAR with CFS-PML and regular PML

<table>
<thead>
<tr>
<th>Frequency</th>
<th>D (cells)</th>
<th>Variation in SAR [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 MHz</td>
<td>4</td>
<td>-2</td>
</tr>
<tr>
<td>1 GHz</td>
<td>4</td>
<td>-2</td>
</tr>
<tr>
<td>2 GHz</td>
<td>4</td>
<td>-2</td>
</tr>
<tr>
<td>5 GHz</td>
<td>4</td>
<td>-2</td>
</tr>
</tbody>
</table>

*Note: D denotes the thickness of the PML.*
unlike the regular PML, which produced large error especially at the lower frequencies. The width of the CPML was relatively small in the above calculations, and it could be easily increased, which would make the error even smaller. In many practical calculations, such as this one, even a relatively thin 5-cell CPML might give good enough results.

4.2. Box phantom

The results of the simulations with the box phantom are presented in figures 5–7. Width of the CPML is six cells in all simulations, and, unless otherwise stated, CFS-PML is used.

Figure 5 shows the performance of CFS-PML at various frequencies. The resolutions for 100 MHz, 1 GHz, 2 GHz and 5 GHz are 6 mm, 2 mm, 1 mm and 1 mm, respectively. Similarly to the case of small sphere, the variation is very small for all frequencies. The weakest performance seems to happen at 2 GHz.

The effects of FDTD mesh resolution on the performance of the CFS-PML are studied in the 1 GHz and 2 GHz cases. The results are illustrated in figure 6, where the variation in SAR values is calculated relative to the 1 mm resolution result. As can be seen in the figures, the same CFS-PML performs very well for all the studied resolutions. The variations of SAR values with the distance to PML are insignificant compared to uncertainties due to resolution, e.g. at 2 GHz, the maximum error due to PML is approximately 0.25%, but using 2 mm resolution instead of 1 mm causes almost 3% lower SAR values. Using 3 mm resolution causes even larger error, because the ‘ten cells per wavelength’ rule of thumb is not satisfied inside the muscle.
The 2 GHz case with 1 mm resolution was studied further for regular PML and CFS-PML with different values of $\alpha_{\text{max}}$. The width of the CPML was six cells. Figure 7 shows the variation of maximum SAR in the box for regular PML and CFS-PML for different values of $\alpha_{\text{max}}$. For regular PML, ten cells are sufficient to guarantee that the error in SAR$_{\text{wb}}$ is smaller than 0.5%. This is again much better than reported in Wang et al (2006). In this case, $\alpha_{\text{max}} = 0.05$ or $\alpha_{\text{max}} = 0.10$ seems like the best choice. When $\alpha_{\text{max}} = 0.20$, the error varies sinusoidally, which implies a slightly too large $\alpha$, so that the absorption of propagating waves is weakened.

4.3. Realistic human body model

The results of the simulations with the NORMAN phantom are presented in tables 2 and 3 at 300 MHz and 2.14 GHz, respectively. The PML width is six cells in all results, and the power density of the incident plane wave is normalized to 1 W m$^{-2}$ (rms). As can be seen, the variation in both the whole-body and 10 g-averaged SAR is very small for both frequencies. While the variation of SAR values is very small for both CFS-PML and regular PML individually, CFS-PML gives average 0.7% and 1.0% higher whole-body and 10 g SAR values than regular PML at 300 MHz. These slight differences might be caused by the different
performances of the two PMLs, but which PML is the most accurate remains unclear. For 2.14 GHz, the average differences are smaller: negligible for whole-body SAR and −0.4% for 10 g SAR.

These results support the conclusions in Findlay and Dimbylow (2006), i.e. the variation of SAR values is very small even for the regular PML in the case of a full-sized human body model. It seems that for such a large problem, the fields are only weakly evanescent, so using regular PML instead of CFS-PML may be sufficient.

5. Discussion

When observing the presented variations of SAR values with the object–PML distances, one can derive some basic rules for error analysis. It seems that the variation can be divided
roughly into a sum of two components, an exponentially decaying component and a sinusoidal component, which apparently correspond to the reflection errors due to evanescent fields and propagating fields, respectively. This can be seen clearly in figure 7: for small $\alpha$, when evanescent fields are reflected, the error seems purely exponential; and for large $\alpha$, when the absorption of propagating waves is weak, the error is almost sinusoidal. In most other results, both components are present. Naturally, the form of these variations is problem specific, and these observations might not hold for special geometries.

It seems very natural that the exponential component of the variation is due to the reflection of evanescent waves, as the evanescent fields decay exponentially with the distance to the object. Exponential part cannot necessarily be removed by increasing the PML width as the reflection occurs at the air–PML interface (Bérenger 1999). Thus, when using regular PML, a sufficiently thick free-space layer is needed around the object. Another, a less memory-demanding, option is to replace regular PML with CFS-PML (such as CPML), which may be used to eliminate the exponential part of the error almost completely, as seen in, e.g., figures 3(a) and (b). For regular PML, this part of the error seems to be concentrated on the lower frequencies. This can be explained by the form of the coordinate stretching variables (1): when the frequency $\omega$ is low, the influence of $\alpha$ is large. At higher frequencies, the significance of $\alpha$ decreases, and regular PML performs better. This might explain why the error in SAR values is slightly larger at lower frequencies in Findlay and Dimbylow (2006).

The sinusoidally varying component, which is most likely due to the reflection of propagating waves, decays slowly with the PML–object distance. It can be reduced by increasing the width of the PML or reducing $\alpha$, which improve absorption of propagating waves. The effects of increasing the PML width can be seen clearly in the CFS-PML curves in figures 3(b)–(d). The effects of reducing $\alpha$ to make the sinusoidal part smaller can be seen in figure 7.

In the sphere simulation in Wang et al (2006), the error is more sinusoidal than exponential, which implies it is caused more by insufficient absorption of propagating waves rather than evanescent fields. A properly implemented 12-cell UPML should be able to absorb propagating waves very well, so it seems there might be an error in the implementation of UPML in that paper. As such, increasing the free-space-layer width reduces the error only a little. The actual error due to too small PML–sphere distance, i.e. the error due to evanescent waves, should decay much faster, and be completely negligible for large distances.

6. Conclusions

The performance of CPML absorbing boundary conditions in FDTD SAR calculations was studied. In some cases, the regular PML may not be sufficient, and CFS-PML is needed to ensure that no additional free-space layers are needed between the object and the PML, e.g. in the case of small sphere or muscle box, the benefits of CFS-PML compared to the regular PML were clear. However, based on the results presented here and in Findlay and Dimbylow (2006), the regular PML seems to function sufficiently well for the SAR analysis of a full-sized human body model under plane-wave exposure. In such cases, the PML could be placed very close to the model without noticeable error.

The performance of PML depends on the problem, but often there seems to be no need to tune the PML parameters for each problem separately, e.g. for the CFS-PML studied in this work, the same parameters worked well for a variety of cases, including different frequencies, resolutions, problem geometries and CPML widths. Also, a very thick PML was unnecessary, as 6-cell CPML gave already very good results.
Based on the presented results, the conclusion is that well-implemented CPML, using the CFS-PML approach, guarantees that no additional free-space layers are needed around the phantom, and that the numerical uncertainty due to PML is negligibly small. Such CFS-PML seems to be better suited for a general SAR assessment problem than regular PML, which did not function as well in all situations. However, it seems that the performance of regular PML should still be much better than that reported in Wang et al (2006).

Acknowledgments

We would like to thank Dr Peter Dimbylow, the Health Protection Agency, UK, for providing the NORMAN phantom. Financial support received from TEKES (Finnish Funding Agency for Technology and Innovation) and the Nokia Corporation is acknowledged.

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