Reliable FDTD simulation convergence detection and acceleration

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Introduction: Finite-difference time-domain (FDTD) simulations [1] are an important tool for RF engineers and are routinely employed in the MR coil building process to assist in design choices and safety evaluation (SAR) [2]. The simulation process can be regarded as calculating the impulse response of the coil structure in question: An input pulse is fed to the coil port and its energy is distributed throughout the system and dissipates in lossy structures or is radiated into the far field. During this process, the values of the electric and magnetic fields are sampled according to the Nyquist theorem and consecutively (or on-the-fly) undergo a discrete Fourier transform for the frequency(s) of interest to obtain S-Parameters and field distributions. An important criterion for the accuracy of the results is the level of convergence: If the simulation is terminated too early, the impulse response is only partially sampled, leading to potentially wrong results. Most commercial solvers employ the remaining energy content of the system (given in dB w.r.t. the maximum value) as a measure of convergence. Since this is an abstract value, it does not provide immediate insight as to how large the truncation error might be, leading to a disagreement in the community on a sensible convergence level. Moreover, structures like birdcage coils exhibit multiple resonant modes with Q-factors (corresponding to mode "lifetime") much higher than the mode of interest. The total energy content of the system can be dominated by these modes, concealing the convergence of the interesting mode and significantly prolonging the simulation. While this can be circumvented by choosing an input pulse of small bandwidth, one has to keep in mind that a small bandwidth equals a long pulse; and depending on the mode frequency spacing an appropriate pulse length for suppression of unwanted modes may well dominate the simulation time. In this work, we aim to present a way to directly inspect the level of convergence at a given frequency and minimize the simulation time for multimode structures.

Methods: A time-domain signal a is sampled N times with a time step of Δt. Its Fourier component $F(f)$ at frequency f can be calculated using the equation $F(f) = \sum_{n=0}^{N} a(n) \cdot \exp(-2\pi i \cdot f \cdot n \cdot \Delta t)$. Regarding the sum as cumulative, that is looking at the sequence $F(f)_{|N=0\ldots N}$, one can monitor the temporal evolution of the Fourier component during the sampling process. While memory constraints do not permit the inspection of the whole three-dimensional volume in this manner, it is sufficient to observe a few points of interest and especially the port signals, since these are responsible for a correct power scaling. An analysis of the resulting curves yields insight into the convergence behavior of the model: If the mode of interest has decayed sufficiently, the time derivative of F will approach zero and the simulation can safely be terminated. Oscillations indicate the presence of other modes that have not yet fully decayed and thus exhibit the characteristic side lobes of a harmonic signal truncated with a rectangular window function. The amplitude of these oscillations depends on the local energy density and spectral distance of the leaking modes from the observed frequency. By applying a suitable apodization function to the time domain signals as soon as the mode of interest is decayed, the leakage could be sufficiently suppressed and the simulation terminated early without having to resort to unwieldy pulse lengths. The approach was tested on a 3T highpass birdcage resonator simulated in XFdtd 7.2 (Remcom, State College, PA, USA) with a broadband excitation (up to 1 GHz).

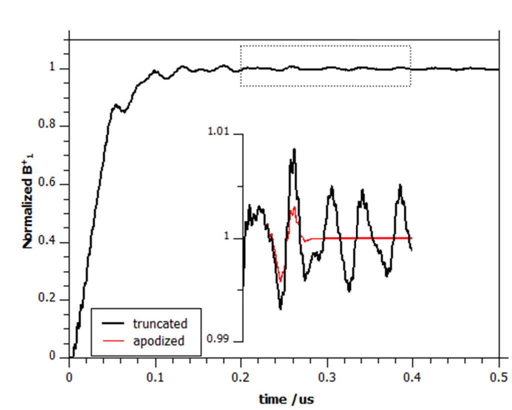

Fig. 1: Evolution of the central B_1^+ value at 124 MHz

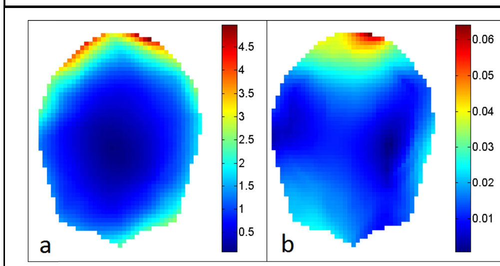

Fig. 2: Truncated (a) and apodized (b) deviations of the B_1^+ distribution from the fully converged values (central axial slice) in percent

Results: An example for the temporal evolution of the center B_1^+ value at the imaging frequency of a 3T birdcage resonator is given in Fig. 1. After approximately 0.3 µs, the imaging mode is fully decayed and the aforementioned oscillatory behavior from the higher order modes is visible. XFdtd reports a convergence level of only -4 dB which is far from the minimum advisable level of -30 dB as suggested in the manual. Yet, the maximum error when truncating at this point stays below 1% and below 5 % for the complete central axial slice (Fig. 2a). Applying a cos² shaped apodization function between 0.2 µs and 0.3 µs will reduce the already small error by almost two orders of magnitude (Fig 1, Fig. 2b). Further precision enhancement can be achieved by starting the apodization at a later time and prolonging the apodization interval.

Conclusion: The results suggest that the total remaining energy is not a suitable indicator for the convergence MR resonators with multiple modes. Rather, the convergence of the fields inside the object of interest (e.g. phantom, human model) at a specified frequency should be monitored. Our approach allows to directly examine the errors introduced by early termination of the simulation. An implementation of apodization routines into commercial FDTD solvers could yield time savings without sacrificing any accuracy.

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