Chapter 25
FDTD Method and HPC for Large-Scale Computational Nanophotonics

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Abstract From 2010 to 2014 the number of papers using the Finite-Difference Time-Domain (FDTD) method for nanophotonics has doubled (from more than 700 to 1430 papers – Google Scholar, searching "FDTD and nanophotonics"). The simulation of the light-matter interaction at the nano-scale requires very fine mesh-sizes to capture the physics, as for example in nanoplasmonics. Large computational resources are needed to achieve a good accuracy, and not taking care of that could result in non-convergent or inaccurate calculations. The availability of a high-performance computing (HPC) system (a massively parallel IBM Blue Gene/Q of the Southern Ontario Smart Computing Innovation Platform – SOSCIP) allows us to perform high-resolution simulations otherwise impossible using an in-house parallel 3D-FDTD code. Here we demonstrate the convergence of the FDTD method simulating the interaction of a linearly-polarized plane-wave with a gold nanosphere of radius 60 nm in the range 400–700 nm. The full study is reported in (Calà Lesina et al., On the convergence and accuracy of the FDTD method for nanoplasmonics, Opt Exp 23(8), 2015). The problem of the scattering of a plane-wave by a sphere is analytically known from the Mie theory. Varying the mesh size down to the limit allowed by the supercomputer, which has 65,536 cores, the numerical results are compared to the analytical ones. This study can be considered as a guideline for a proper FDTD simulation setup.

In Fig. 25.1 we use per-component mesh, double-precision, and Drude+2CP. A mesh size of 0.5 nm is required to get an average percentage error <*%err*> less than 1 %. In Fig. 25.2 we use uniform staircase mesh; we observe a slower convergence. In Fig. 25.3 we use single-precision; we observe divergences due to accumulating round-off errors. In Fig. 25.4 we use the standard Drude model which do not model the interband transitions.

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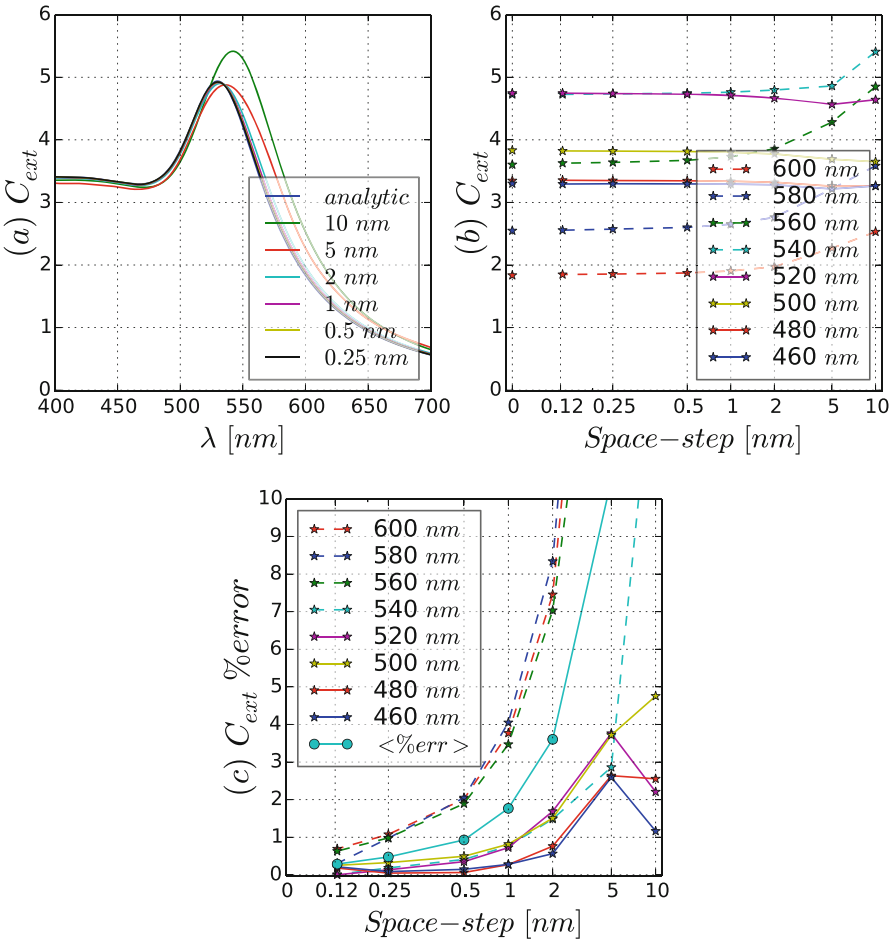

Fig. 25.1 Gold sphere C_{ext} convergence study: (**a**) and (**b**) spectra, (**c**) percentage error. Reference simulation setup: per-component mesh, double precision, and Drude+2CP model

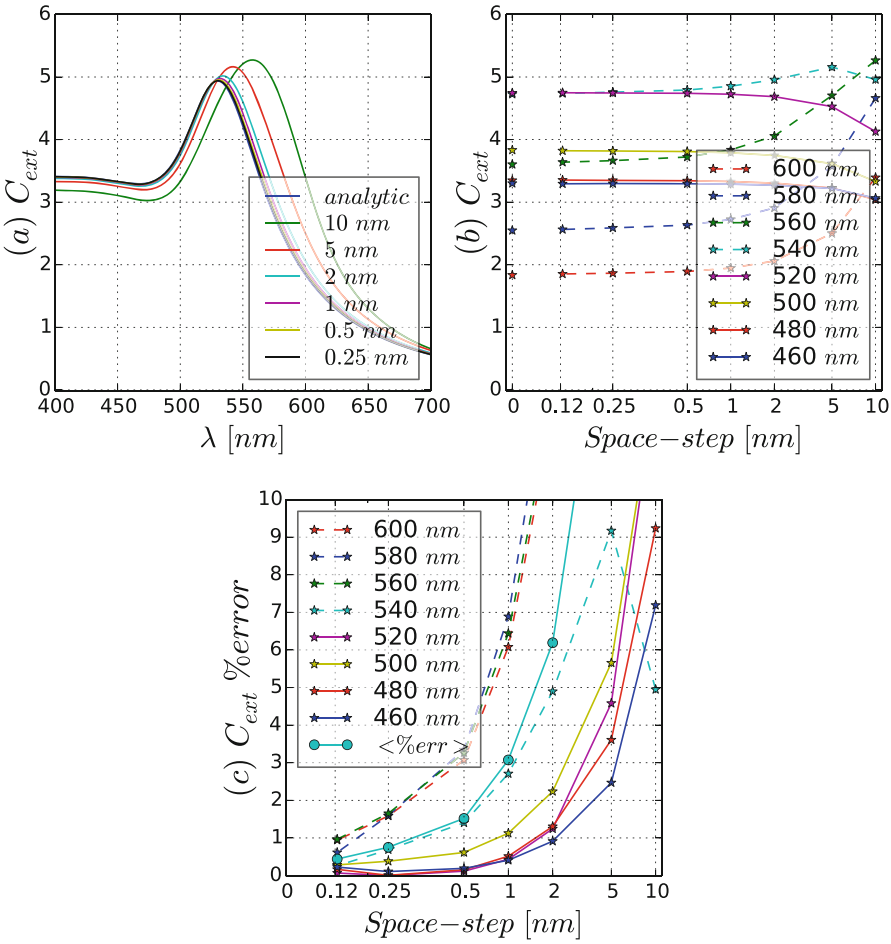

Fig. 25.2 Gold sphere C_{ext} convergence: (**a**) and (**b**) spectra, (**c**) percentage error. Simulation setup as in Fig. 25.1, except uniform staircase

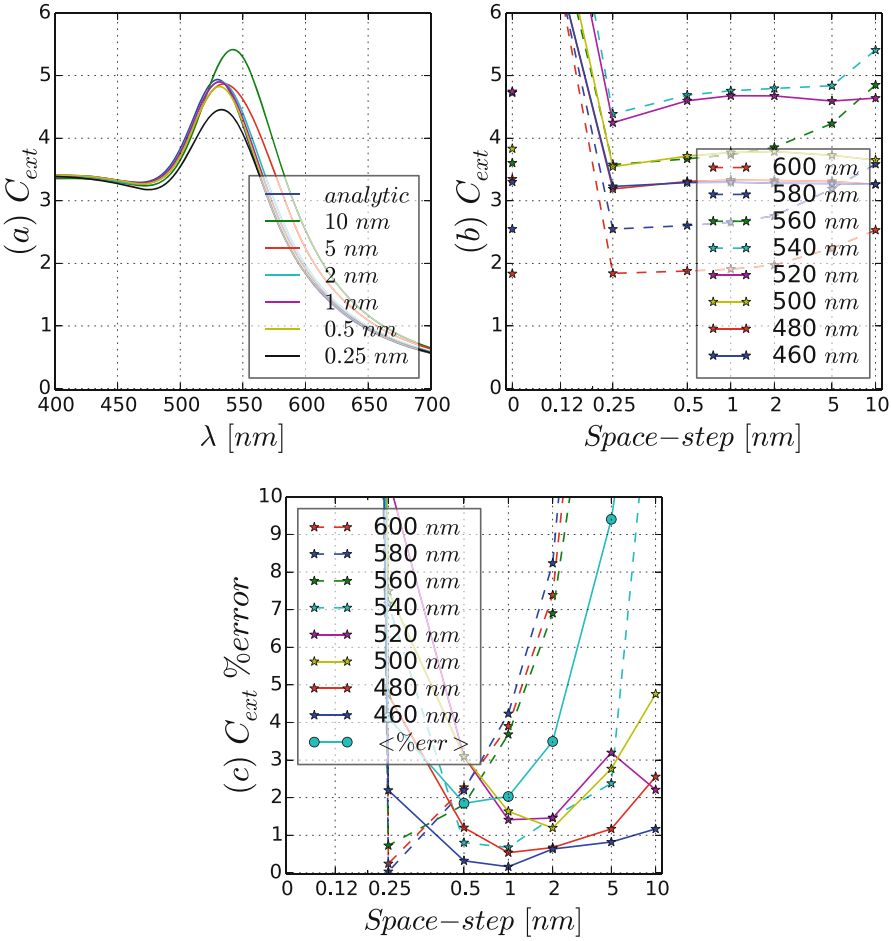

Fig. 25.3 Gold sphere C_{ext} convergence: (**a**) and (**b**) spectra, (**c**) percentage error. Simulation setup as in Fig. 25.1, except single-precision

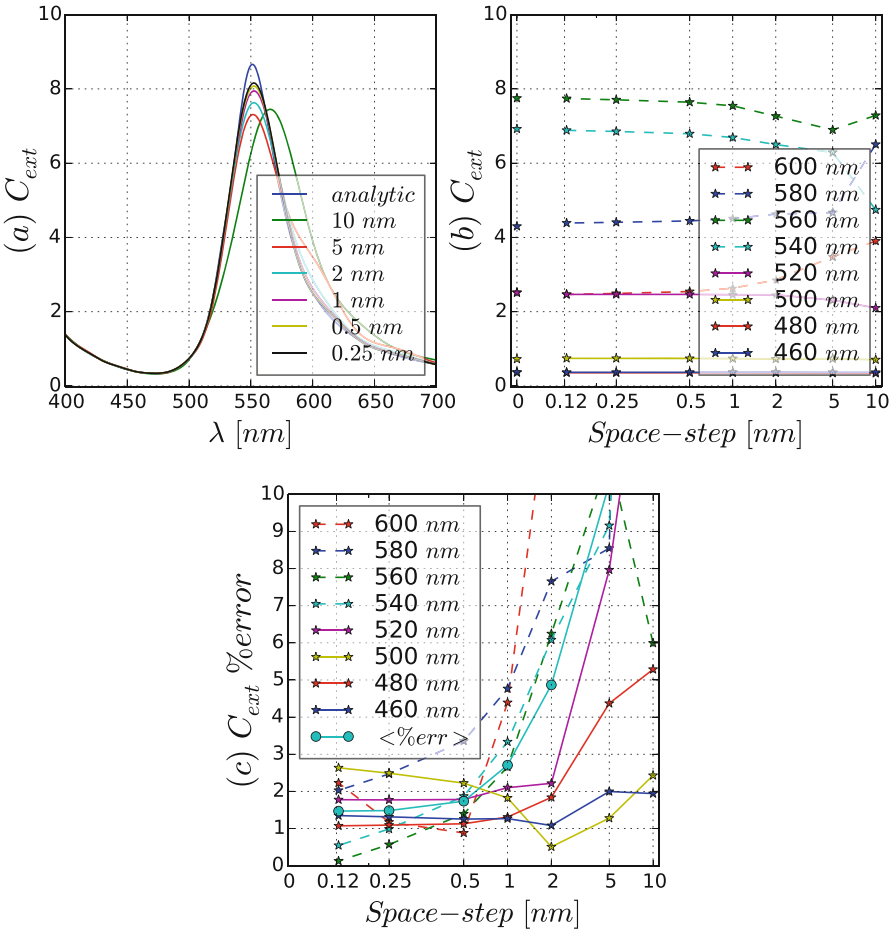

Fig. 25.4 Gold sphere C_{ext} convergence: (**a**) and (**b**) spectra, (**c**) percentage error. Simulation setup as in Fig. 25.1, except standard Drude model