0.0.1 Simulation of beam propagation in the Fraunhofer regime

Purpose: This exercise illustrates numerical difficulties in FFT-BPM propagation in far field. Concretely, we look at:

a) how cyclic (periodic) boundary conditions imposed by the Fourier transform prevent a truly long-distance simulated beam propagation,

b) simple numerical technique of a boundary guard, which is a kind of "poor-man's" method to mimic transparent boundary conditions at the computational box edge,

a) and effects of grid-resolution in the spectral domain, that show up especially in case of an initial condition with sharp edge(s).

The most important lesson of this exercise is that while such "poor man‘s" transparent boundary conditions can be fully sufficient in some cases, one must be always rather careful and look out for numerical artifacts introduced due to the modified boundary.

Task: Calculate the Fraunhofer diffraction pattern of a simple slit through the FFT-based beam propagation. The aim of this exercise is to explore a situation which "amplifies" certain numerical issues connected with FFT-BPM, and beam propagation in general.

Solution:

There are three Matlab scripts, *pFarField_1.m*, *pFarField_2.m*, and *pFarField_3.m* in this exercise package. They are essentially identical, provided for easy comparison of different simulation regimes. The situation simulated represents the Fraunhofer diffraction on a one-dimensional slit. The diffracted field is propagated sufficiently far, so that an approximation of the far-field Fraunhofer pattern is obtained.

Script *pFarField_1.m* utilizes a sufficiently large computational domain, and the boundary-guard is not used. This example shows that a reasonable approximation of the far-field pattern can be obtained if the domain is sufficiently large, and its spatial resolution is fine enough. Of course, it makes the computation relatively expensive. Here, in this one-dimensional case it may not be an issue, but it can in general (especially in two dimensions and in time-dependent problems) make the simulation prohibitively expensive.

This motivates script *pFarField_2.m* which is an attempt to achieve far field simulation with a smaller domain. Inspection of the boundary region in the simulated beam profile at the final distance reveals artifacts that are due to wings of the pattern coupling back because of the cyclic boundary conditions imposed by the FFT method.

Script *pFarField_3.m* switches on the boundary guard. It is designed to eliminate the problem with the periodic domain boundaries. Readers should inspect the script to see what implementation of the guard was chosen, and experiment with its settings.

In general, one has to choose the thickness of the boundary-guard layer. This is a part of the domain that is essentially "sacrificed," and not useful for obtaining any information form the simulated solution. Another parameter of the guard is the steepness with which its absorption increases toward the edge of the domain. If it is too steep, it can itself induce strong reflection, and thus make the domain effectively smaller.

By playing with these characteristics, it should be easy to realize that this way of handling the unwanted “reflections” from the boundaries is a rather subtle business. The take-away lesson is that with these simple boundary conditions, one has to pay keen attention to possible numerical artifacts.

One could say that the remedies we have used to improve the fidelity of our simulation on a smaller lattice were designed to control waves with extreme transverse wavenumbers. These are the components of the solution that propagate at steepest angles, and therefore experience first the finite size of the computational domain. In line with the observations made in one-dimensional Maxwell solver, it is the waves which belong to the edges of the resolved numerical bandwidth that tend to cause problems.

Note: An alternative way to deal with the extreme wavenumbers in the beam propagation is to design a propagator that will damp all waves with wavenumbers higher than a chosen threshold. This can be realized as a boundary guard in the spectral domain. Similar to the situation in the real space, the transition between the unperturbed and damped regions of transverse wavenumbers must be sufficiently gradual. If this transition is sharp, wave-forms arise in the real space representation that exhibit long non-decaying “tails,” with characteristic wavenumbers, namely those separating the damped and un-damped wave-vectors.