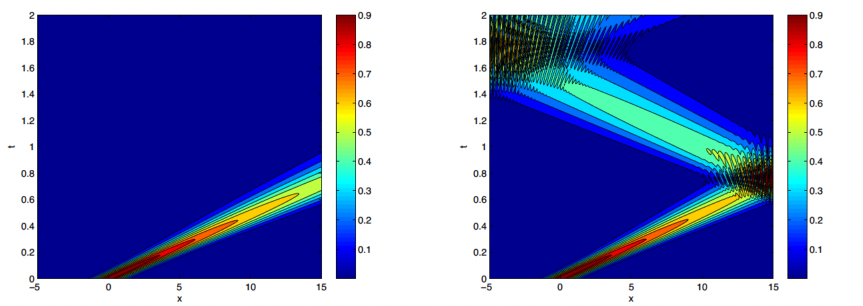
On boundary conditions for numerical solutions of quantum wave equations

M2 MSIAM - Modeling seminar

Keywords: wave mechanics; absorbing boundary conditions; perfectly matched layers; Schrödinger equation; Dirac equation; numerical schemes.

Project description: Wave mechanics is a branch of quantum physics in which the behaviour of objects (such as elementary particles) is described in terms of their wavelike properties. In this context, Partial Differential Equations (PDE) such as Schrödinger, Klein-Gordon or Dirac equations can be considered. They govern the time evolution of the wave function associated to a quantum system.

For numerical simulations, PDEs have to be solved in a bounded spatial domain. Since the wave propagation is a physical phenomenon that is not confined within a bounded domain, the choice of boundary conditions is a crucial issue as illustrated in Figure 1. The objective is to build artificial boundary conditions that accurately approximate the exact solution in the whole space domain. Among the techniques that exist in the literature, we will discuss on the so-called Absorbing Boundary Conditions (ABCs) and Perfectly Matched Layers (PMLs).



(a) Exact reference solution

(b) Numerical solution with a Dirichlet boundary condition

Figure 1: Example coming from [1] for an exact solution of a 1D Schrödinger equation (left) and a numerical solution imposing unsuited boundary conditions that generate some spurious unphysical reflections (right).

The first part of this project will be devoted to the Schrödinger equation in order to get familiar with this equation in its simplest form and the numerical schemes that are usually used to discretize it. Then, we will consider the derivation and the discretization of ABCs and PMLs as described in the recent review [1] and references therein. The objective is to implement and compare different approaches. Depending on the progression, other quantum wave equations will be also considered.

Prerequisites: M1 PDE course, basics on numerical analysis, Python programming.

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References

[1] X. Antoine, E. Lorin, and Q. Tang, "A friendly review of absorbing boundary conditions and perfectly matched layers for classical and relativistic quantum waves equations," *Molecular Physics*, vol. 115, no. 15-16, pp. 1861–1879, 2017.