Approximate boundary conditions for nonlinear Schrödinger equations and applications to computational methods.

In many applications, and most particularly in the case of dispersive equations, the (system of) PDE(s) that must be numerically solved is set in an unbounded spatial domain. This is for example the case of the time dependent Schrödinger equation that arises in laser modeling and quantum physics. However, this situation is also met for example for the KdV or Davey-Stewartson equations. In view of a numerical treatment, one must truncate the spatial domain into a bounded one that we call Ω here. Of course, to get a solvable problem, a boundary condition must be imposed on the associated nonphysical fictitious boundary $\Sigma = \partial\Omega$. This problem is better known as building *artificial or absorbing boundary conditions* (ABCs) for PDEs.

In the case of the Schrödinger equation that can be considered as a model problem, serious developments related to ABCs have been proposed. Even for the simplest prototype, the one-dimensional linear constant coefficients Schrödinger equation, both the theoretical construction and the numerical discretization of the ABCs are nontrivial. Indeed, in this case, the ABC, that can be written through the Dirichlet-to-Neumann (DtN) operator, involves fractional derivative operators that must be carefully discretized to get fully unconditionally stable schemes. In the case of higher dimensions, variable coefficients and nonlinear problems, the theoretical developments require the use of much more advanced mathematical techniques, basically pseudodifferential and microlocal analysis methods.

We will present the usual methods to determine ABC for nonlinear Schrödinger equation in one and two dimensional setting. We will also address the question of approximation of the nonlocal Dirichlet-to-Neumann operators and present numerical simulations.

References

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