WORKSHOP
Waves, boundaries and oscillations in numerical schemes
Rennes, November 2-4 2016

Schedule

Wednesday November 2nd

13h30 - 14h30	Pascal Noble (INSA Toulouse) *Discrete transparent boundary conditions for KdV-BBM equations*
14h30 - 15h30	Sonia Fliss (ENSTA ParisTech) *Transparent boundary conditions for the wave equation in infinite complex media*
15h30 - 16h00	break
16h00 - 17h00	Erwan Faou (INRIA Rennes) *On travelling wave for the discrete nonlinear Schrödinger equation*
17h00 - 18h00	Benjamin Boutin (Rennes) *Numerical boundary layers for linear hyperbolic IBVP and semigroup estimate*

Thursday November 3rd

9h00 - 10h00	Anton Arnold (TU Wien) *Open boundary conditions for wave propagation problems on unbounded domains.* I
10h00 - 10h30	break
10h30 - 11h30	Christian Rohde (Stuttgart) *Numerical computation of nonclassical shock waves in multiple space dimensions*
11h30 - 12h30	Hermen Jan Hupkes (Leiden) *Discretization schemes vs travelling waves for bistable reaction-diffusion systems*
12h30 - 14h00	lunch
14h00 - 15h00	Anton Arnold (TU Wien) *Open boundary conditions for wave propagation problems on unbounded domains.* II
15h00 - 15h30	break
15h30 - 16h30	Loïc Le Treust (Marseille) *Uniformly accurate splitting methods for the semiclassical limit of the Schrödinger equation*
16h30 - 17h30	Rémi Carles (CNRS & Montpellier) *Time splitting methods and the semi-classical limit*
20h00	dinner

Friday November 4th

9h00 - 10h00	Anton ARNOLD (TU Wien) *A hybrid WKB-based method for highly oscillatory ODEs in the semi-classical limit*
10h00 - 10h30	break
10h30 - 11h30	Gautier DAKIN (CEA) *High-order discretization of boundary conditions for hyperbolic system on Cartesian grids*
11h30 - 12h30	Arnaud DURAN (Lyon) *Low Froude number schemes for the multi-layer shallow water system*
12h30 - 14h00	lunch

Abstracts

A. ARNOLD

First topic : *Open boundary conditions for wave propagation problems on unbounded domains*

We shall first review the basic principles and the construction of various open boundary conditions (absorbing BCs, perfectly matched layers). Then we focus on transparent boundary conditions (TBCs) for the time-dependent Schrödinger equation (in 1D and for waveguide geometries). The discretization of such TBCs may raise stability issues. This may be coped with by preserving structural properties of the continuous problem in the discrete scheme (e.g. L^2 preservation).

Discrete TBCs for the Schrödinger equation are non-local in time, and hence computationally expensive. We shall derive approximate discrete TBCs, obtained by a discrete sum-of-exponential approximation of the convolution kernel (for the Schrödinger equation in 1D and for a circular geometry).

As another example we shall discuss a discrete TBC for the 1D Dirac equation, discretized by a staggered-grid leap-frog scheme. An important prerequisite for the stability of the scheme with TBCs is the monotonicity preservation of the dispersion relation in the whole space scheme (avoiding the notorious *fermion doubling*).

Second topic : *A hybrid WKB-based method for highly oscillatory ODEs in the semi-classical limit*

We are concerned with the efficient numerical integration of ODEs of the form $\epsilon^2\psi_{xx} + a(x)\psi = 0$ for $0 < \epsilon << 1$ (appearing as a stationary Schrödinger equation or 1D Helmholtz equation, e.g.) on coarse grids, but still yielding accurate solutions. In two steps we derive an accurate finite difference scheme that does not need to resolve each oscillation:

a) With a WKB-ansatz the dominant oscillations are "transformed out", yielding a much smoother ODE.

b) For the resulting oscillatory integrals we devise an asymptotic expansion both in ϵ and h.

In contrast to existing strategies, the presented method has (even for a large spatial step size h) the same weak limit (in the classical limit $\epsilon \to 0$) as the continuous solution. Moreover, it has an error bound of the order $O(\epsilon^3 h^2)$. Also, we shall give extensions to k.p-Schrödinger systems, turning points (using an Airy function ansatz), and the numerical coupling of the highly oscillatory regime (i.e. for given $a(x) > 0$) with evanescent regions (i.e. for $a(x) < 0$). In the oscillatory case we use a marching method that is based on an analytic WKB-preprocessing of the equation. And in the evanescent case we use a FEM with WKB-ansatz functions.

We present a full convergence analysis of the coupled method, showing that the error is uniform in ϵ and second order w.r.t. h. We illustrate the results with numerical examples for scattering problems for a quantum-tunnelling structure.

B. BOUTIN : *Numerical boundary layers for linear hyperbolic IBVP and semigroup estimate*

The study concerns the one-dimensional scalar transport equation on the half real line, when considering the homogeneous Dirichlet condition at the boundary. In the framework of finite difference schemes with arbitrarily many time levels, we construct and analyze the numerical boundary layers. Under classical consistency and stability assumptions for the discrete Cauchy problem and an additional technical assumption on the non-decreasing oscillating patterns, the two-scale boundary layer expansion yields a close to optimal discrete semigroup estimate.

R. Carles : *Time splitting methods and the semi-classical limit*
We consider the time discretization based on Lie-Trotter splitting, for the nonlinear Schrödinger equation, in the semi-classical limit, with initial data under the form of WKB states. Both the exact and the numerical solutions keep a WKB structure, on a time interval independent of the Planck constant. We prove error estimates, which show that the quadratic observables can be computed with a time step independent of the Planck constant. We give a flavor of the functional framework, based on time-dependent analytic spaces.

G. Dakin : *High-order discretization of boundary conditions for hyperbolic system on Cartesian grids*
A new high-order discretization of boundary conditions for hyperbolic systems on Cartesian grids is proposed. The main difficulties reside in the fact that the control volumes do not coincide with the geometry of the problem. The method is based on Inverse Lax-Wendroff procedure for the prescribed boundary conditions. High-order accurate ghost values of conservative variables are imposed using Taylor expansion. The method is fully detailed in the linear case and stability analysis is performed. The corner stone of the algorithm is the inversion of a system (linear or non-linear) which is well-posed in all our examples. Numerical examples are given for the linear case and for the Euler equation in 1D and 2D.

A. Duran : *Low Froude number schemes for the multi-layer shallow water system*
This work is mainly concerned with stability issues in connection with the design of numerical schemes for the multi-layer shallow water system, in view of applications in large scale oceanography. Two criteria are in use in such regimes, namely the fact that the mechanical energy should be nonincreasing (entropic schemes) and the consistency with low Froude number regimes that are observed at the continuous level (asymptotic preserving schemes). We shall see how, starting from a new interpretation of the model at the continuous level, we can achieve those two objectives in various contexts (explicit, semi-implicit, staggered grids).

E. Faou : *On travelling wave for the discrete nonlinear Schrödinger equation*
I will discuss the possible existence of travelling wave solutions in discrete nonlinear Schrödinger equations on a grid. I will show the influence of the nonlinearity in this problem and give some partial results. This is joint work with Dario Bambusi, Joackim Bernier, Benot Grébert and Alberto Maspero.

S. Fliss : *Transparent boundary conditions for the wave equation in infinite complex media*
We are interested in acoustic or elastic wave propagation in time harmonic regime in a two-dimensional medium which is a local perturbation of an infinite anisotropic homogeneous and/or periodic medium. We investigate the question of finding artificial boundary conditions to reduce the numerical computations to a neighborhood of this perturbation. This question is difficult due to the anisotropy and/or the periodicity of the surrounding medium. Our approach consists in coupling several semi-analytical representations of the solution in half-planes surrounding the defect with a FE computation of the solution around the defect. The difficulty is to ensure that all these representations match, in particular in the infinite intersections of the half-planes. It leads to a formulation which couples, via integral operators, the solution in a bounded domain including the defect and its traces on the edge of the half-planes.

H. J. Hupkes : *Discretization schemes vs travelling waves for bistable reaction-diffusion systems*
We study various temporal and spatial discretization methods for bistable reaction-diffusion problems, including adaptive grids. The main focus is on the functional differential operators that arise after linearizing around travelling waves in various well-understood limits and studying how the subsequent discretization schemes affect the spectral properties of these operators. These represent highly singular

perturbations that we attempt to understand via weak-limit methods based on the pioneering work of Bates, Chen and Chmaj (2003).

L. Le Treust : *Uniformly accurate splitting methods for the semiclassical limit of the Schrödinger equation*

We present new numerical methods for the semiclassical Schrödinger equation. A phase-amplitude reformulation of the equation is described where the Planck constant ε is not a singular parameter. This allows to build splitting schemes whose accuracy is spectral in space, of up to fourth order in time, and independent of ε before the caustics. The second-order method additionally preserves the L^2-norm of the solution just as the exact flow does. We also prove a uniform convergence result for the first-order splitting scheme applied to the linear Schrödinger equation with a potential. Work in collaboration with Philippe Chartier and Florian Méhats.

P. Noble : *Discrete transparent boundary conditions for KdV-BBM equations*

C. Rohde : *Numerical computation of nonclassical shock waves in multiple space dimensions*

Non-Laxian undercompressive shock waves appear in a wide variety of applications that are governed by hyperbolic or hyperbolic-elliptic systems of conservation laws. Examples cover phase boundaries in compressible liquid-vapor flow, martensite-martensite interfaces in metal alloys, or infiltration fronts in immiscible multiphase flow. Most notably, well-posedness of the models can only be reached if additional constraints ?typically in the form of algebraic jump conditions? are prescribed. In the lecture we will first consider an abstract free boundary formulation for undercompressive waves and present some basic well-posedness results including one-dimensional Riemann solvers. In the second part we will address the reliable numerical approximation, which is still a challenging issue, in particular in multiple space dimensions. We will introduce a new class of Finite-Volume methods that are applicable in the latter case. The approach relies on the use of time-dependent meshes which follow the evolution of the non-classical wave front. The local wave front speed is determined from the exact or approximate solution of appropriate Riemann problems. From the analytical point of view we will show that the method is fully conservative, avoids states in the unstable elliptic region, and reproduces planar wave fronts exactly. Moreover, a convergence theorem for the Cauchy problem in one space dimension will be discussed using generalized bounds on the total variation of the approximate solution. Finally, the schemes will be applied to compressible liquid-vapor phase change problems and to overshoot waves in two-phase porous media.