Construction of Transparent Boundary Conditions by the Pole Condition Method

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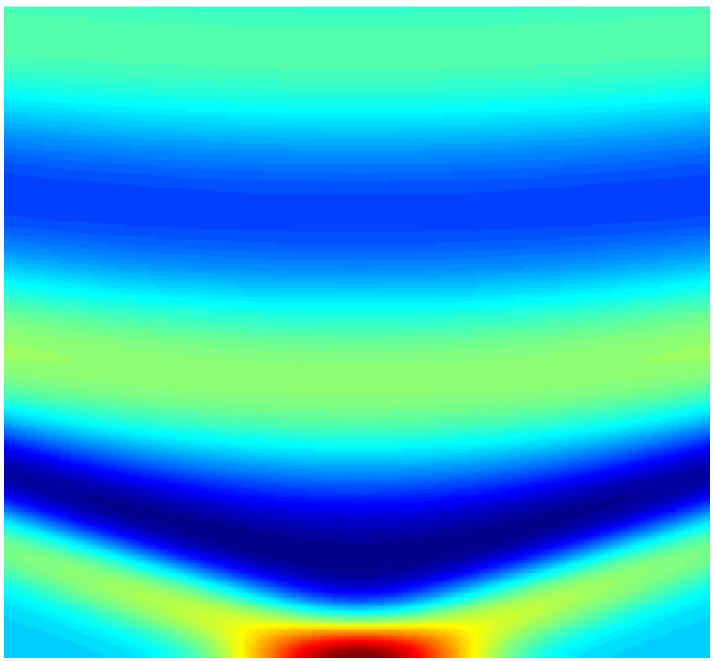


ZIB

Zuse Institute Berlin
Computational Nano-Optics

DFG Research Center MATHEON
Mathematics for key technologies

KAT 7.7

Outline

- Problem classes:
  wave eq., heat eq., drift-diffusion eq., Schrödinger eq.

- Pole condition

- Algorithm

- Convergence

Problem classes

Wave equation

$$\partial_{tt}u(t,x) = \partial_{xx}u(t,x) - k^2(t,x)u(t,x) \quad \text{for } x \in \mathbf{R}, t \geq 0$$

Heat equation/drift – diffusion equation

$$\partial_t u(t,x) = \partial_{xx}u(t,x) + 2d\,\partial_x u(t,x) - k^2(t,x)u(t,x) \quad \text{for } x \in \mathbf{R}, t \geq 0$$

Schrödinger equation

$$i\partial_t u(t,x) = \partial_{xx}u(t,x) - k^2(t,x)u(t,x) \quad \text{for } x \in \mathbf{R}, t \geq 0$$

$$p(\partial_t)u(t,x) = \partial_{xx}u(t,x) + 2d\,\partial_x u(t,x) - k^2(t,x)u(t,x) \quad \text{for } x \in \mathbf{R}, t \geq 0$$

Method

$$p(\partial_t)u(t,x) = \partial_{xx}u(t,x) + 2d\,\partial_x u(t,x) - k^2(t,x)u(t,x) \quad \text{for } x \in \mathbf{R}, t \geq 0$$

↓ Laplace transform in t

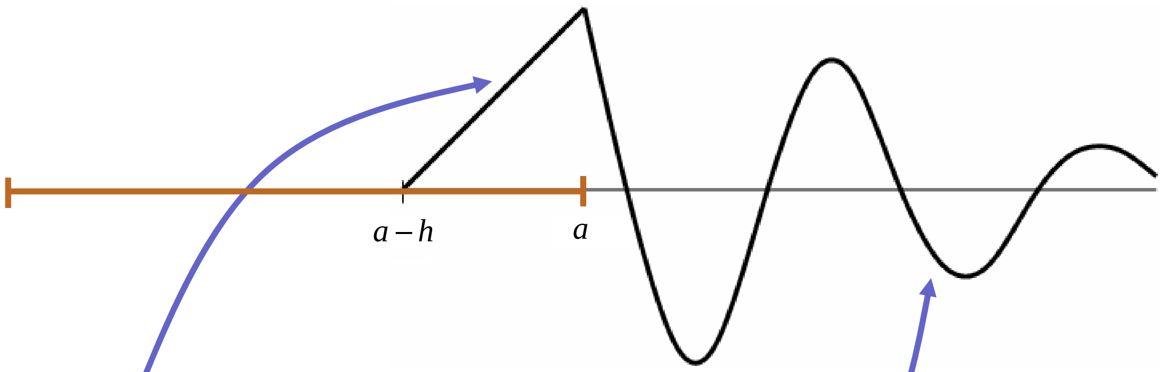
$$p(\omega)\mathbf{u}(\omega,x) = \partial_{xx}\mathbf{u}(\omega,x) + 2d\,\partial_x\mathbf{u}(\omega,x) - K(\mathbf{u})$$

↓ Variational formulation on R

$$\int_{\mathbf{R}} p(\omega)v(x)\mathbf{u}(\omega,x)\,dx = \int_{\mathbf{R}} -\partial_x v(x)\partial_x\mathbf{u}(\omega,x) + 2v(x)d\,\partial_x\mathbf{u}(\omega,x) - v(x)K(\mathbf{u})\,dx$$

Variational formulation on unbounded domain

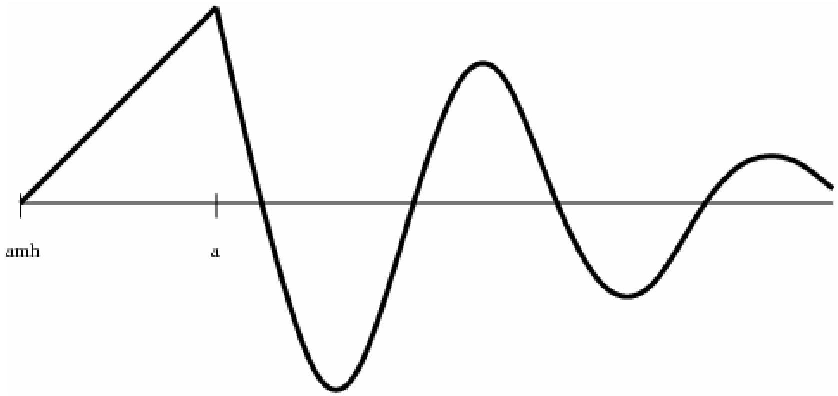
$$\int_{\mathbf{R}} p(\omega) v(x) \mathbf{u}(\omega, x)\, dx = \int_{\mathbf{R}} -\partial_x v(x) \partial_x \mathbf{u}(\omega, x) + 2 v(x) d\, \partial_x \mathbf{u}(\omega, x) - v(x) K(\mathbf{u})\, dx$$



$$v_i = \begin{cases} \max\left(1 - \dfrac{|x - x_i|}{h}, 0\right) : -a \le x \le a \\ \exp(-s(x-a)) : x > a \\ \exp(s(x+a)) : x < -a \end{cases}$$

Laplace transform with respect to distance x

Reinterpretation as Laplace transform



$$\int_{x>a} p(\omega)v(x)\mathbf{u}(\omega,x)\,dx + \int_{a-h}^{a} \ldots dx$$

$$= \int_{x>a} -\partial_x v(x)\partial_x \mathbf{u}(\omega,x) + 2v(x)d\,\partial_x \mathbf{u}(\omega,x) - v(x)K(\mathbf{u})\,dx + \int_{a-h}^{a} \ldots dx$$

$\left(\text{Let } K(\mathbf{u}) = k^2\mathbf{u}\right)$

$$p(\omega)U(\omega,s)$$

$$= s^2U(\omega,s) + 2d\,sU(\omega,s) - k^2U(\omega,s) - r(s,\mathbf{u})$$

Singularities of $U(\omega, s)$

$$p(\omega)U(\omega,s) = s^2 U(\omega,s) + 2d\, sU(\omega,s) - k^2 U(\omega,s) - r(s,\mathbf{u})$$

$$U(\omega,s) = \left(s^2 + 2d\, s - k^2 - p(\omega)\right)^{-1} r(s,\mathbf{u})$$

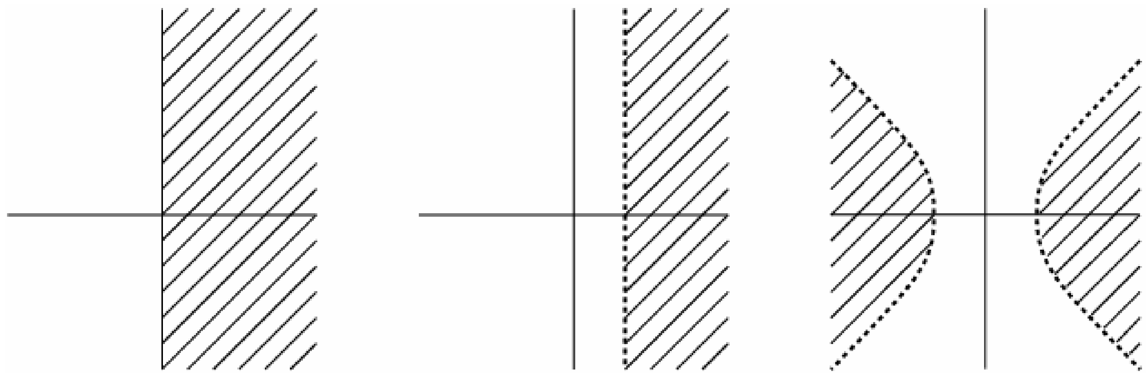
Note: r is a polynom in s

Idea: characterize U by its singularites

Heat equation $p(\omega) = \omega$

$$U(\omega, s) = \left(s^2 + 2d\,s - k^2 - p(\omega)\right)^{-1} r(s, \mathbf{u})$$

possible values | shifted possible values | position of roots

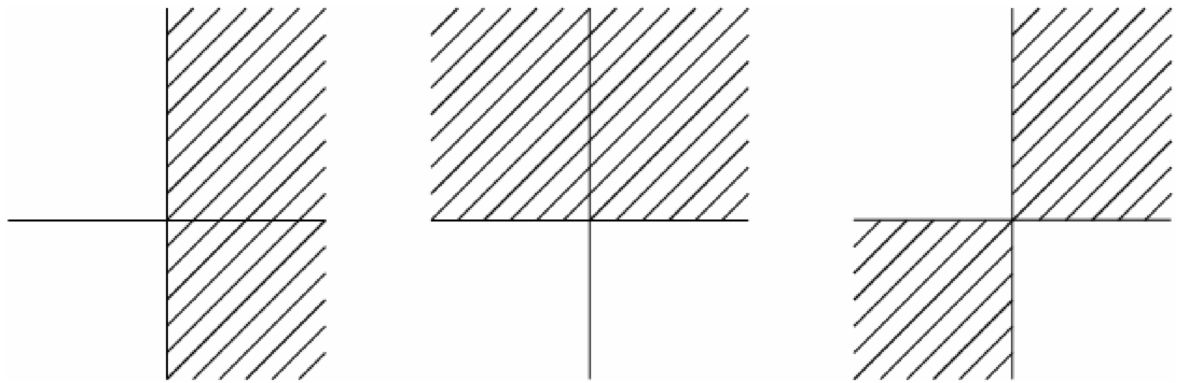


$p(\omega)$ | $p(\omega) + k^2$ | $s_{\pm} = \pm\sqrt{p(\omega) + k^2}$

Schrödinger Equation $p(\omega) = i\omega$

$$U(\omega, s) = \left(s^2 + 2d\,s - k^2 - p(\omega)\right)^{-1} r(s, \mathbf{u})$$

possible values	rotated possible values	position of roots

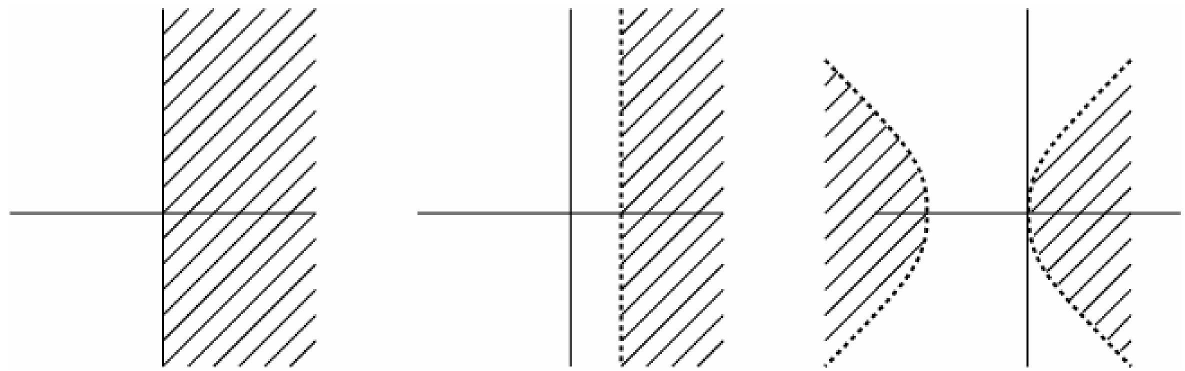


ω	$i\omega$	$s_{\pm}^2 + i\omega = 0$

Drift-Diffusion Equation $\quad p(\omega)=\omega$

$$U(\omega,s)=\left(s^2+2d\,s-k^2-p(\omega)\right)^{-1}r(s,\mathbf{u})$$

possible values | shifted possible values | position of roots

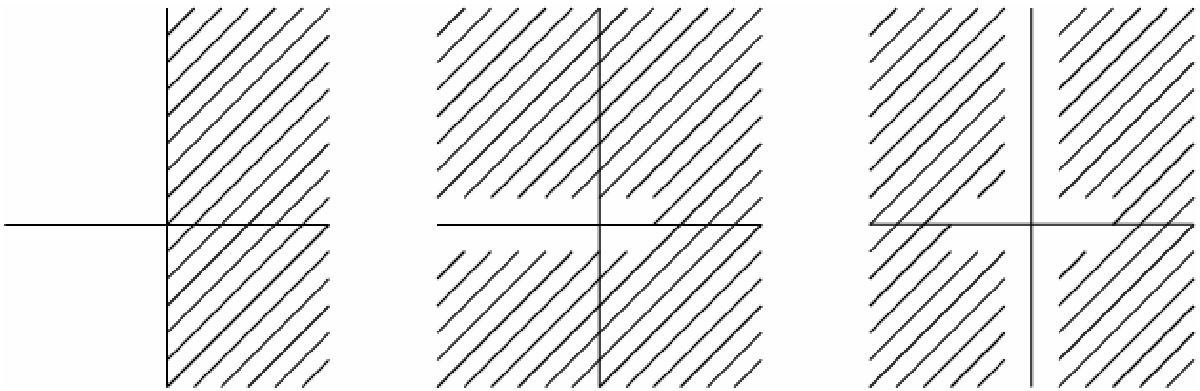


$p(\omega)$ | $p(\omega)+k^2$ | $s_\pm^2+2ds_\pm-\left(p(\omega)+k^2\right)=0$

Wave Equation $p(\omega)=\omega^2$

$$U(\omega,s)=\left(s^2+2d\,s-k^2-p(\omega)\right)^{-1}r(s,\mathbf{u})$$

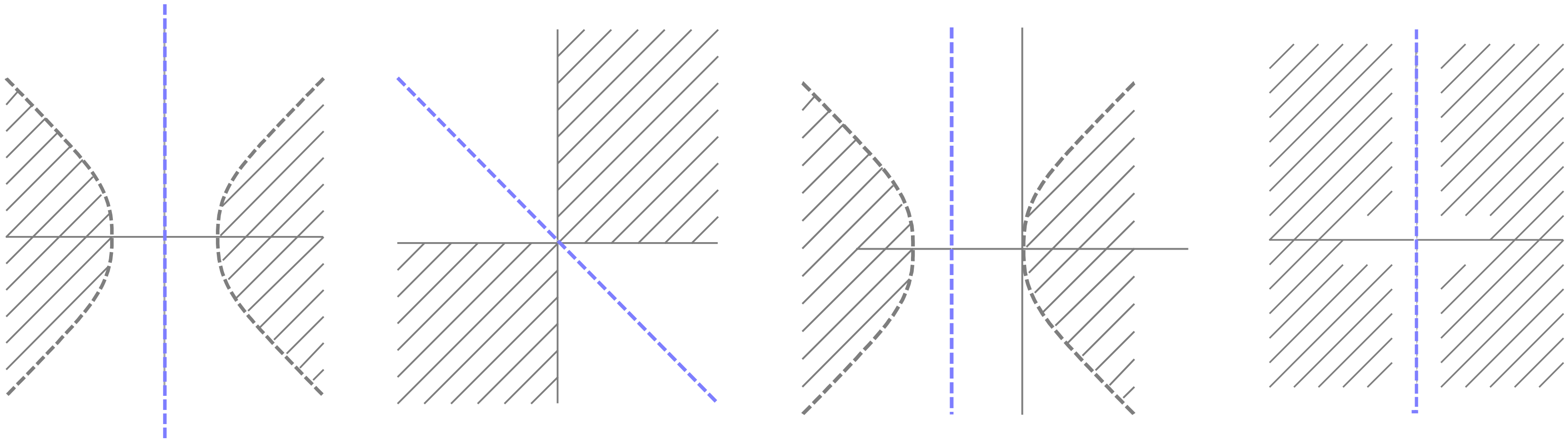
possible values | shifted possible values | position of roots



ω | $p(\omega)+k^2$

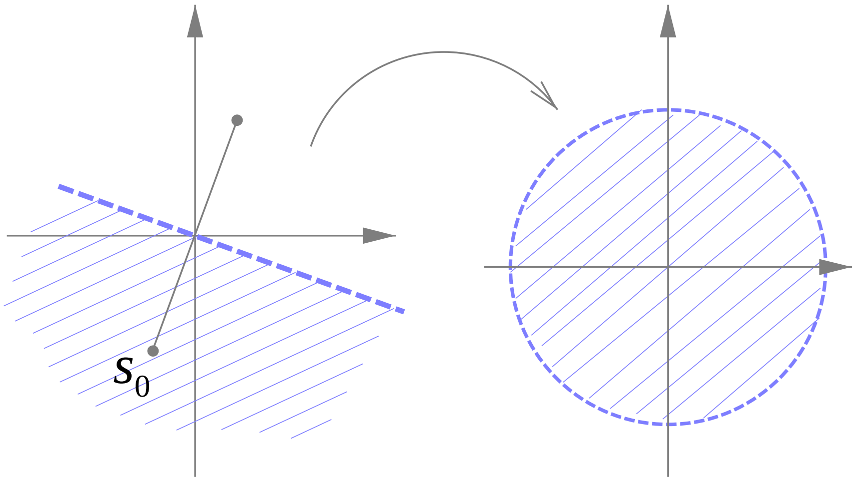
Pole condition

A function $u(\xi,\omega)$ satisfies the pole condition if the Laplace transform of $u(\cdot,\omega)$ has a holomorphic extension to some half-plane H of the complex plane for all ω.



Hardy space approach

Using a Möbius transform the half plane H is mapped to the inner of the unit circle



In the new variable the solution U can be expanded into a power series

$$U(\tilde{s}) = \sum_{n \geq 0} a_n \tilde{s}^n$$

Truncating the power series yields a simple numerical algorithm showing spectral convergence in experiments

Numerical realization: ODE system

From the underlying PDE an ODE system for the Taylor coefficients is obtained:

$$\left(s_0^2 - p - k^2\right)a_0 = u'\big|_\Gamma - s_0 u\big|_\Gamma$$

$$2\left(s_0^2 + p + k^2\right)a_0 + \left(s_0^2 - p - k^2\right)a_1 = -2u'\big|_\Gamma$$

$$\left(s_0^2 - p - k^2\right)a_0 + 2\left(s_0^2 + p + k^2\right)a_1 + \left(s_0^2 - p - k^2\right)a_2 = u'\big|_\Gamma + s_0 u\big|_\Gamma$$

$$\left(s_0^2 - p - k^2\right)a_{l-1} + 2\left(s_0^2 + p + k^2\right)a_l + \left(s_0^2 - p - k^2\right)a_{l+1} = 0, \quad l \geq 2$$

$$s_0 = s_0(\omega) \rightarrow s_0\left(\frac{d}{dt}\right) \qquad p = p(\omega) \rightarrow p\left(\frac{d}{dt}\right) \qquad \rightarrow \text{ODE}$$

Equivalence

For the special choice of the parameter

$$s_0^2 - p(\partial_t) - k^2 = 0$$

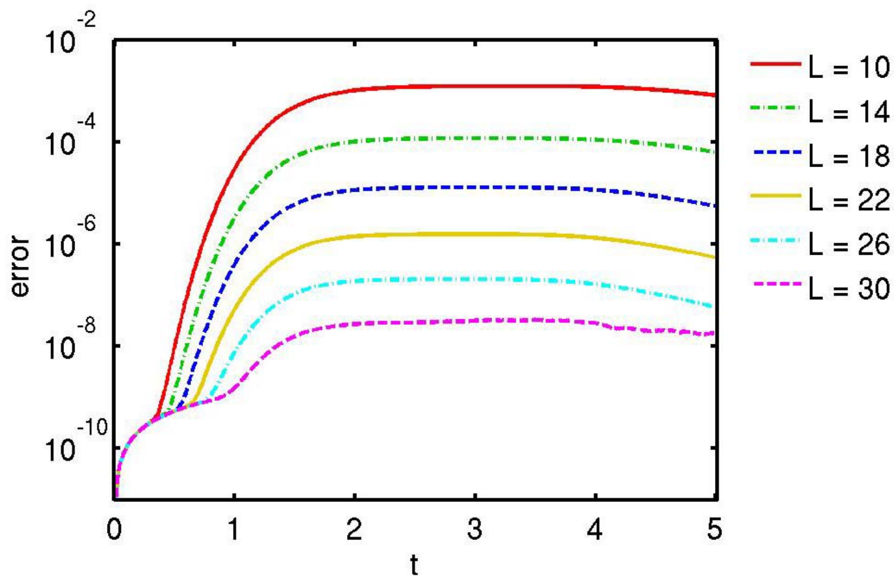
the well-known exact transparent boundary conditions

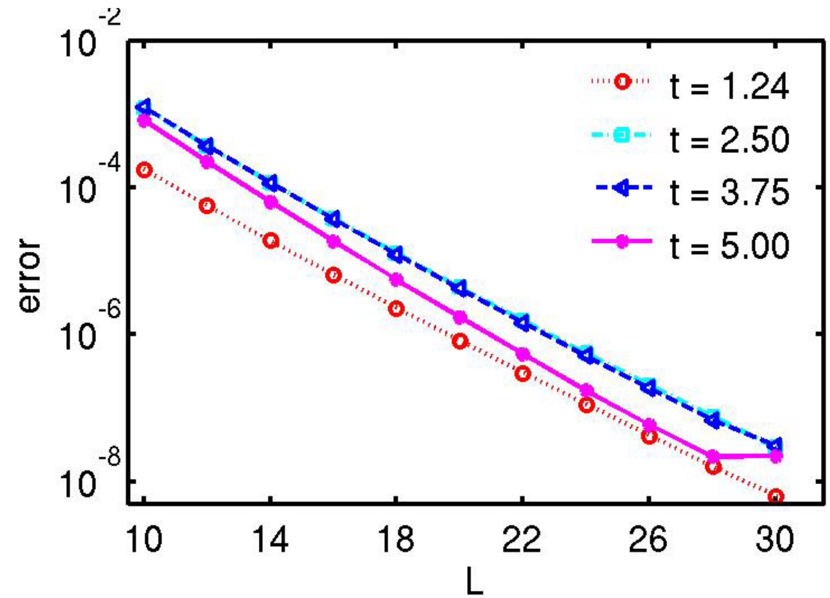
$$0 = u'\big|_\Gamma - s_0 u\big|_\Gamma \quad \Rightarrow \quad u(t)\big|_\Gamma = \int_0^t k(t-\tau)u'(\tau)\big|_\Gamma \, d\tau$$

for a kernel *k* are recovered, where

$$K(\omega) = -\left(p(\omega) + k^2\right)^{-\frac{1}{2}}$$

Schrödinger Equation

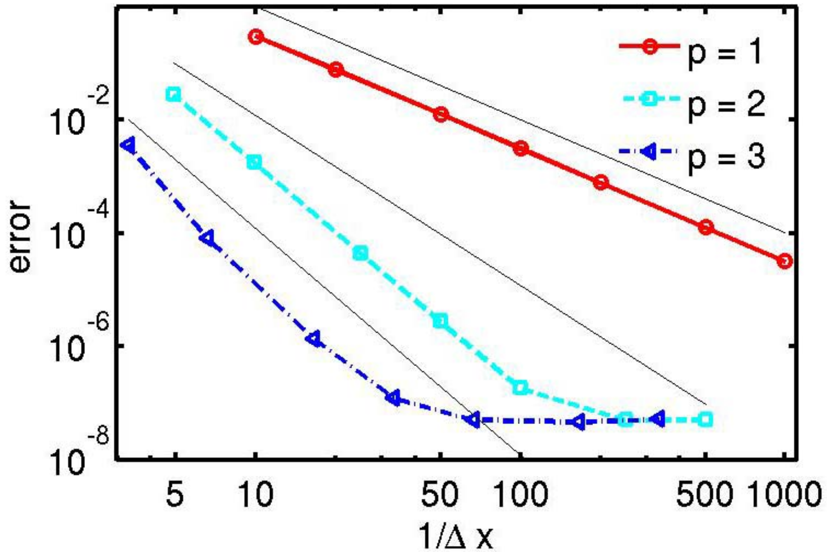


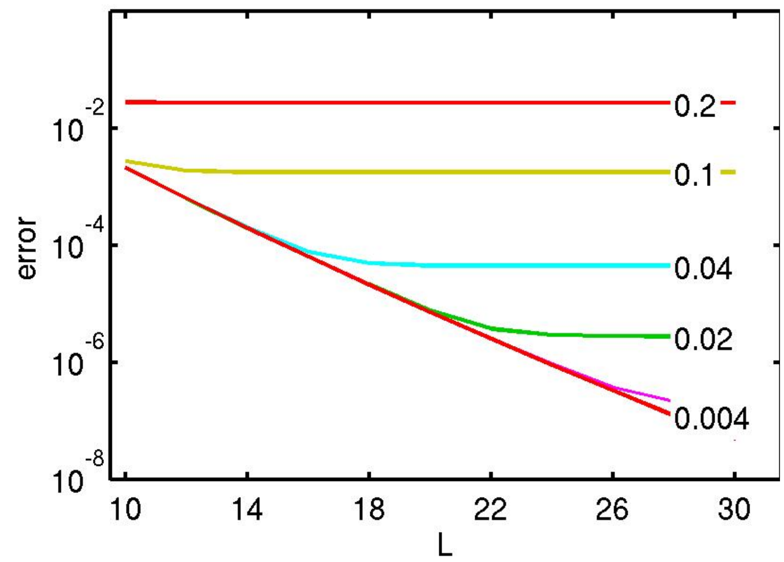


Evolution of the error;
different L, quadratic FEM,
dx = 1/500, dt = 5 · 10−6.

Spatial l2 error at t vs. L;
quadratic FEM,
dx = 1/500, dt = 5 · 10−6.

Schrödinger Equation (2)





Error vs. 1/dx;

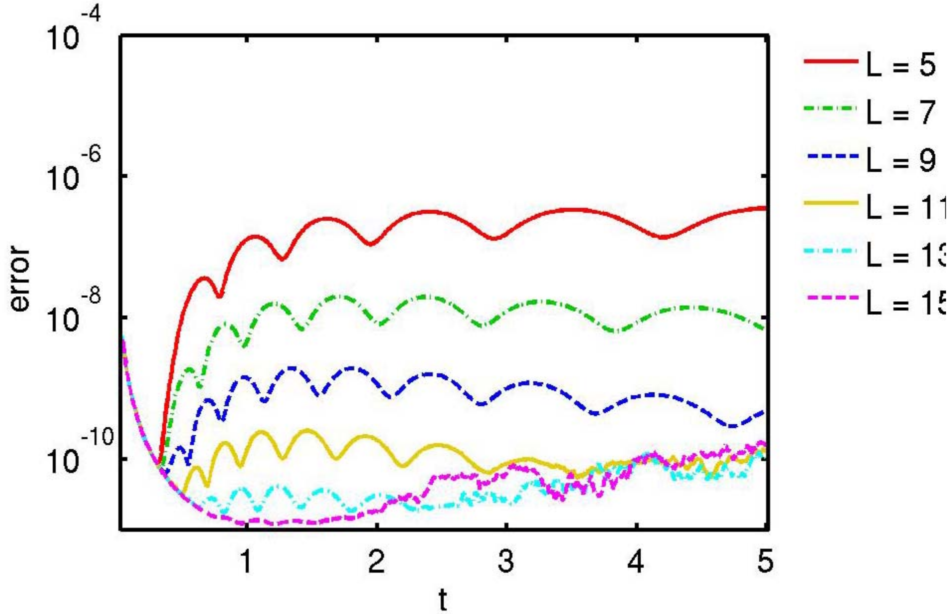
dt = 5 · 10−6, L = 30.

Error vs. L;

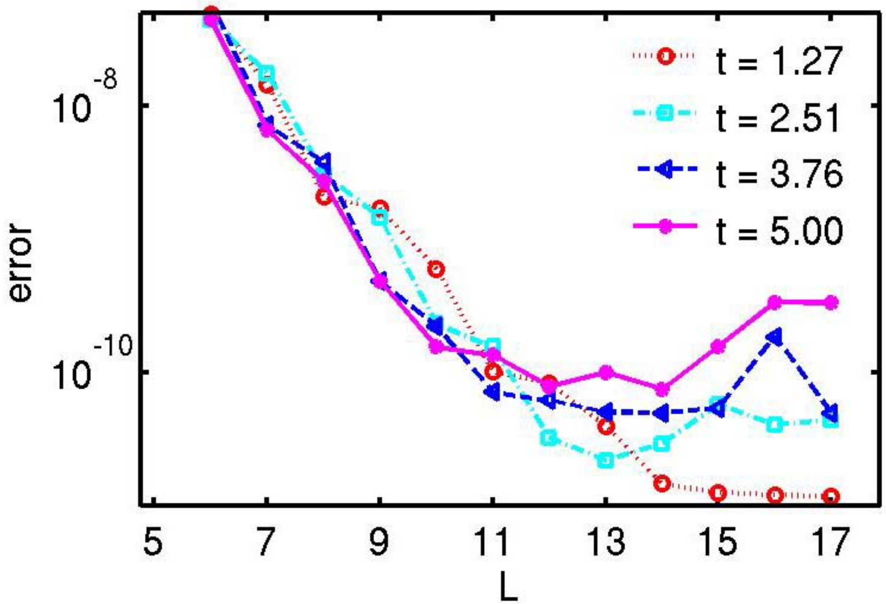
different dx, quadratic FEM,

dt = 5 · 10−6.

Heat Equation

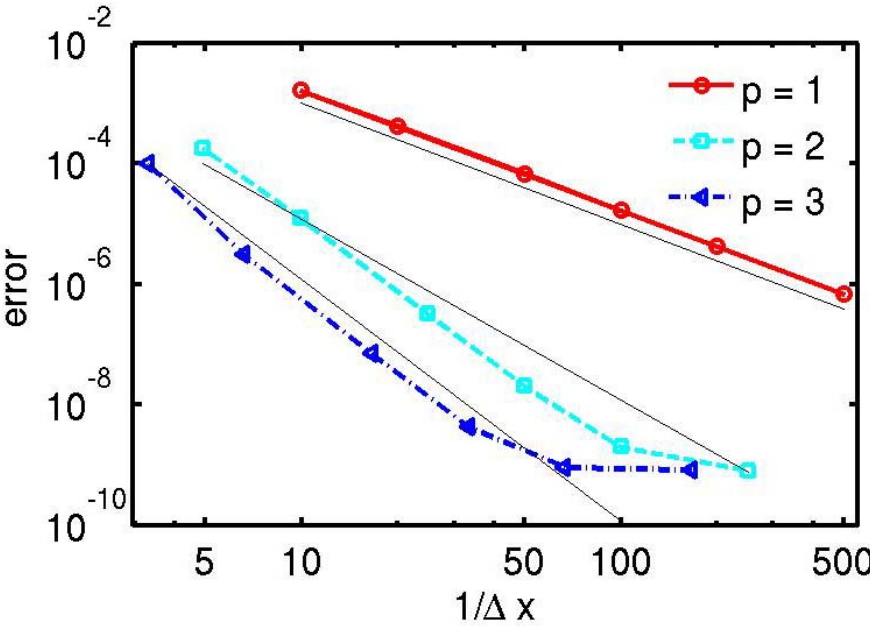


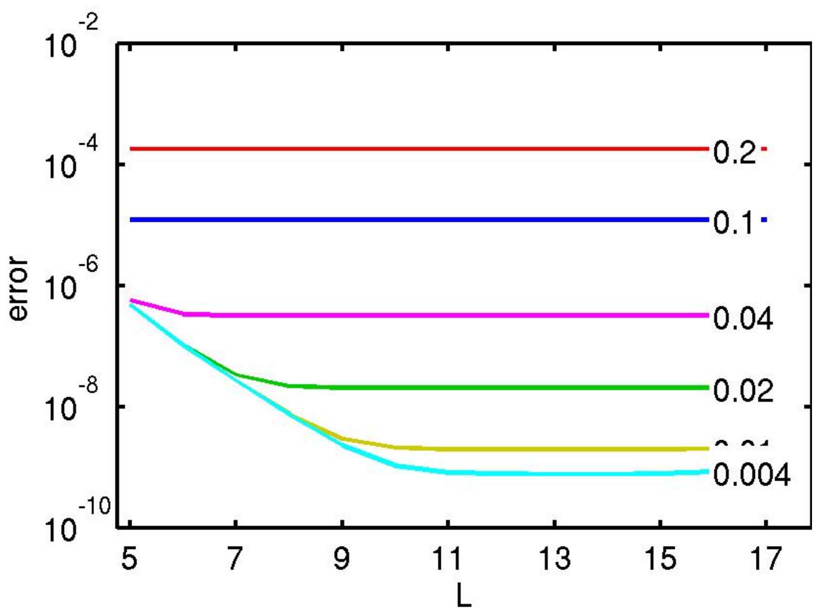
Evolution of the error;
different L, quadratic FEM,
dx = 1/250, dt = 10−5.



Spatial l2 error at t vs. L;
quadratic FEM,
dx = 1/250, dt = 10−5.

Heat Equation (2)

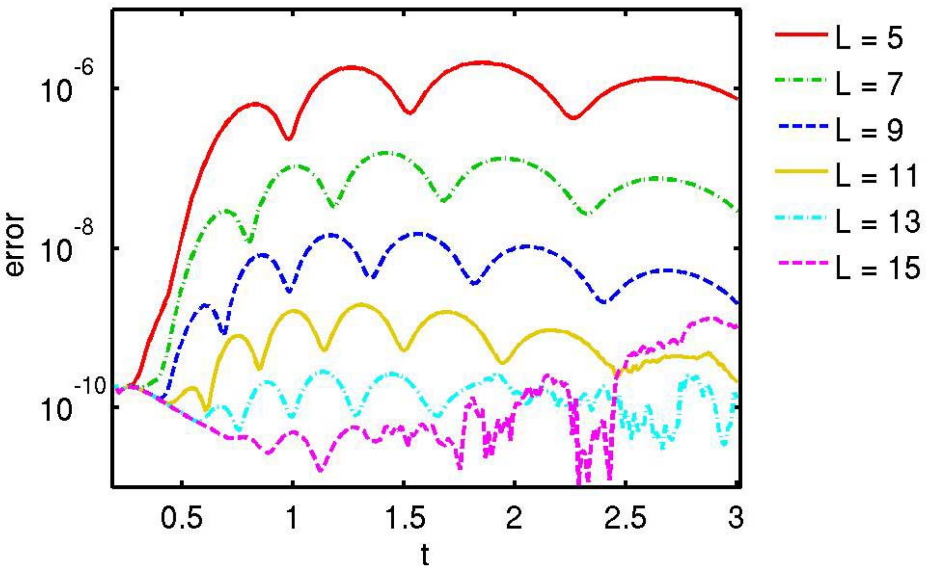


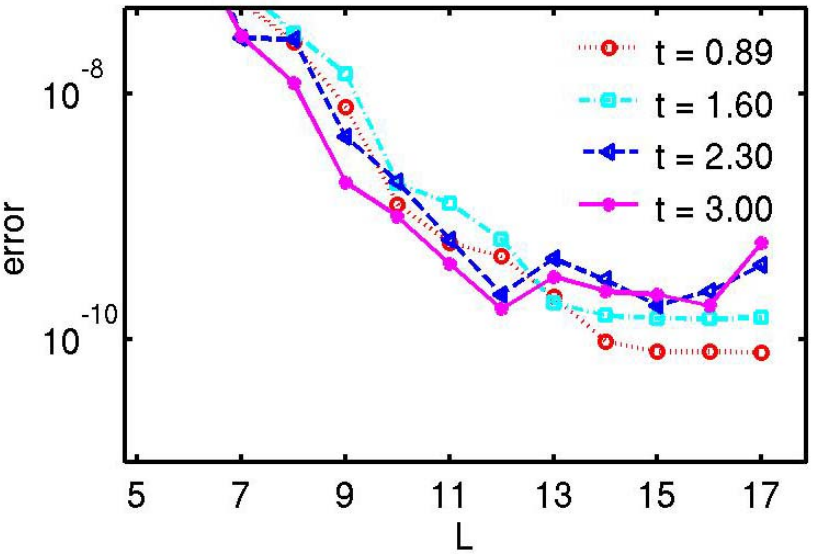


Error vs. 1/x;
dt = 10−5, L = 17.

Error vs. L;
different x, quadratic FEM,
dt = 10−5.

Drift Diffusion Equation

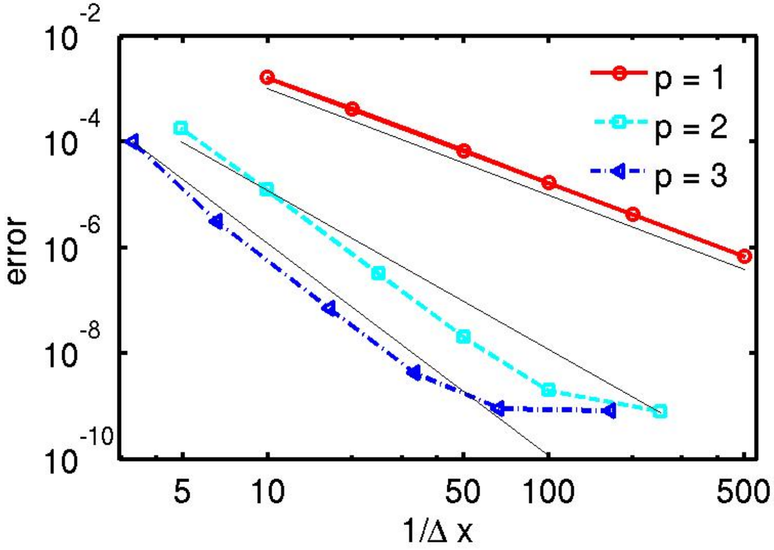


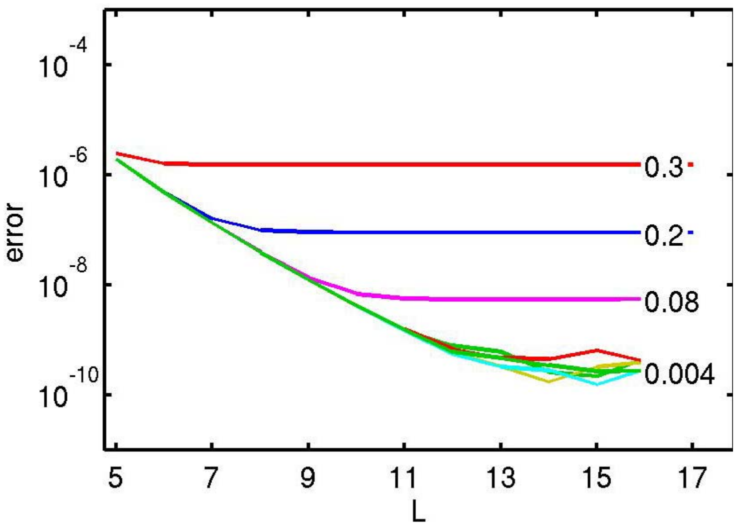


Evolution of l2 error;
different L, quadratic FEM,
dx = 1/400, dt = 10−5..

Spatial l2 error at t vs. L;
quadratic FEM with dx = 1/400
and dt = 10−5.

Drift Diffusion Equation (2)





Error vs. 1/dx;

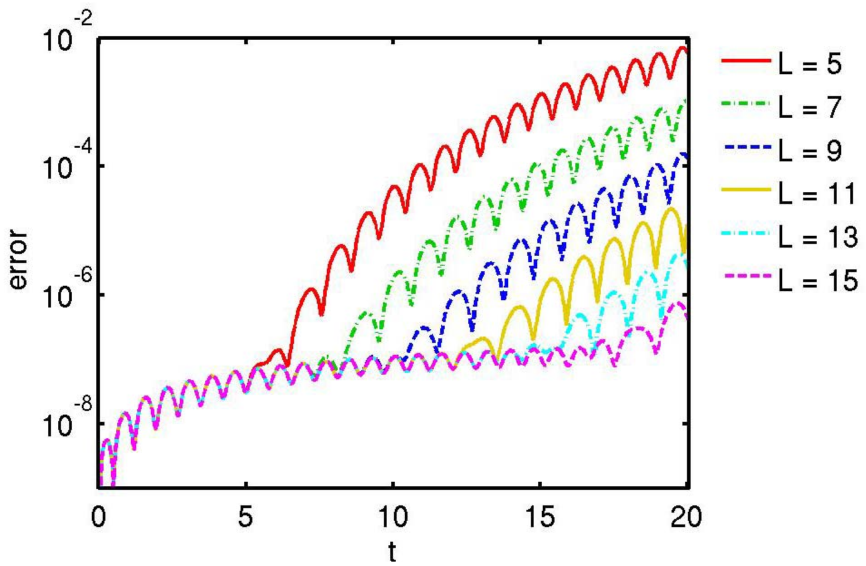
dt = 10−5, L = 17

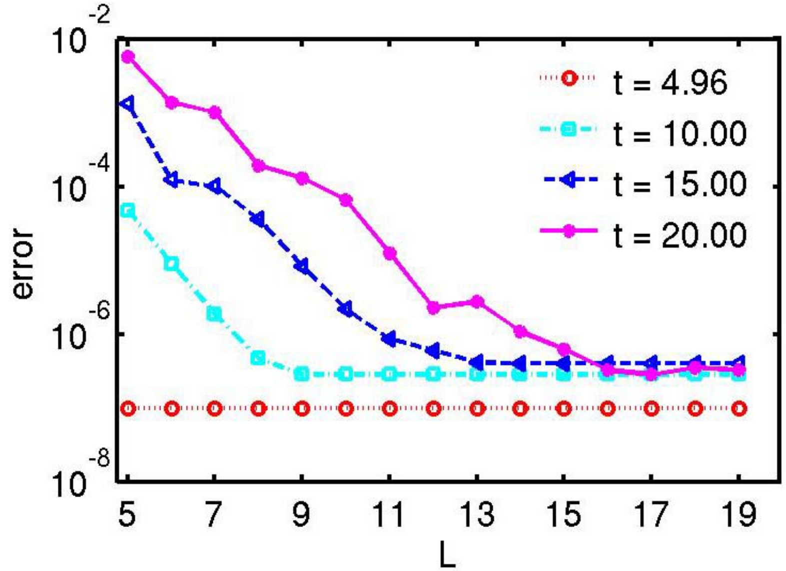
Error vs. L;

different dx, quadratic FEM,

dt = 10−5.

Wave Equation

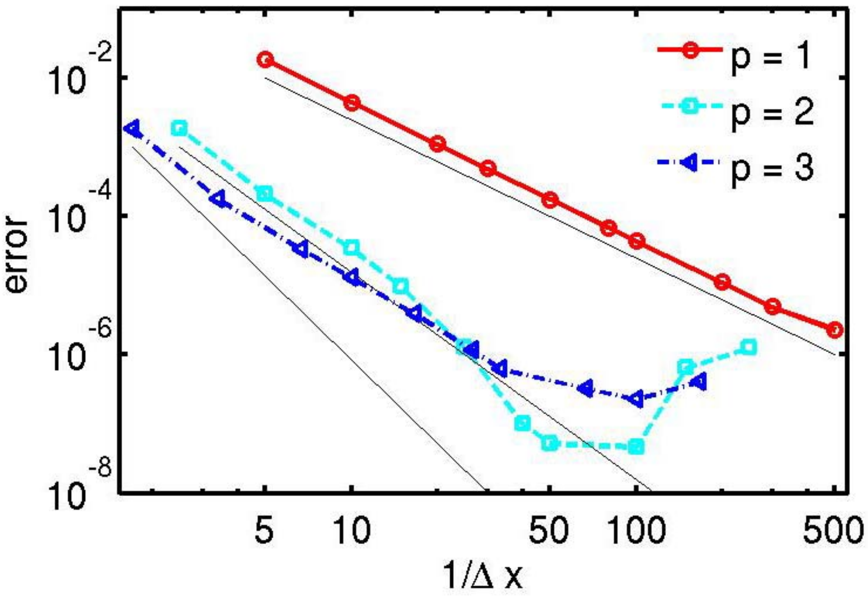


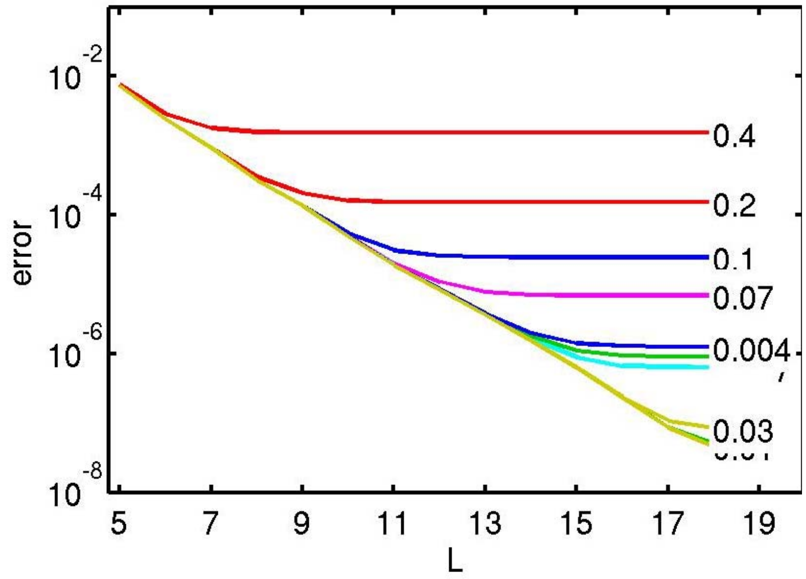


Evolution of the error; quadratic FEM, dx = 1/250, dt = 5 · 10−5.

Error at different t vs. L; quadratic FEM dx = 1/250, dt = 5 · 10−5.

Wave Equation (2)





Error vs. 1/dx;
dt = 5 · 10−5, L = 19.

Error vs. L;
different dx, 2nd order FEM,
dt = 5 · 10−5.

Outlook

- Further types of PDEs (e.g. linear, incompressible, boussinesq gravity waves)
- Systems
- Space dimensions > 1

Summary

- New general approach to the construction of transparent boundary conditions for the wave-, heat-, Schrödinger- and drift-diffusion equation.

- Central idea: The pole condition distinguishes between incoming/unbounded and outgoing/bounded exterior solutions by looking at the poles of the spatial Laplace transform.

- Numerical realization: series representation in Hardy space

- Numerical experiments: in all four equations, the error introduced by the boundary conditions decays exponentially fast in the number L of coefficients