

A Review of Transparent and Artificial Boundary Conditions Techniques for Linear and Nonlinear Schrödinger Equations

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Matthias Ehrhardt

Institut für Mathematik, Technische Universität Berlin

ehrhardt@math.tu-berlin.de

joint work with X. Antoine, A. Arnold, C. Besse and A. Schädle

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Outline

- Numerical Computation on unbounded Domains
- Transparent BCs for the Schrödinger Equation in 1D
 - **Analytic** Transparent BCs
 - **temporally/spatially/fully discrete** Transparent BCs
- Discretizations and Approximations of the Transparent BCs
 - discretization by **quadrature rules**
 - approximation of convolution kernel by sums of exponentials
 - **rational approximations of the Fourier–symbol** of the kernel
- Numerical Example
- Outlook: Cubic nonlinear case

Numerical Computation on unbounded Domains

- Many physical problems are described mathematically by a partial differential equation defined on an **unbounded domain**
- **Numerical computation:** one has to restrict the computational domain Ω by **artificial boundary conditions** or absorbing layers
- If approximate solution coincides on Ω with exact solution, these BCs are called **transparent boundary conditions** (TBCs)
- Constructed artificial boundary conditions should
 - **approximate** the exact whole-space solution restricted to Ω
 - lead to **well-posed** (initial) boundary value problem
 - allow for an **efficient** (and **easy**) numerical implementation

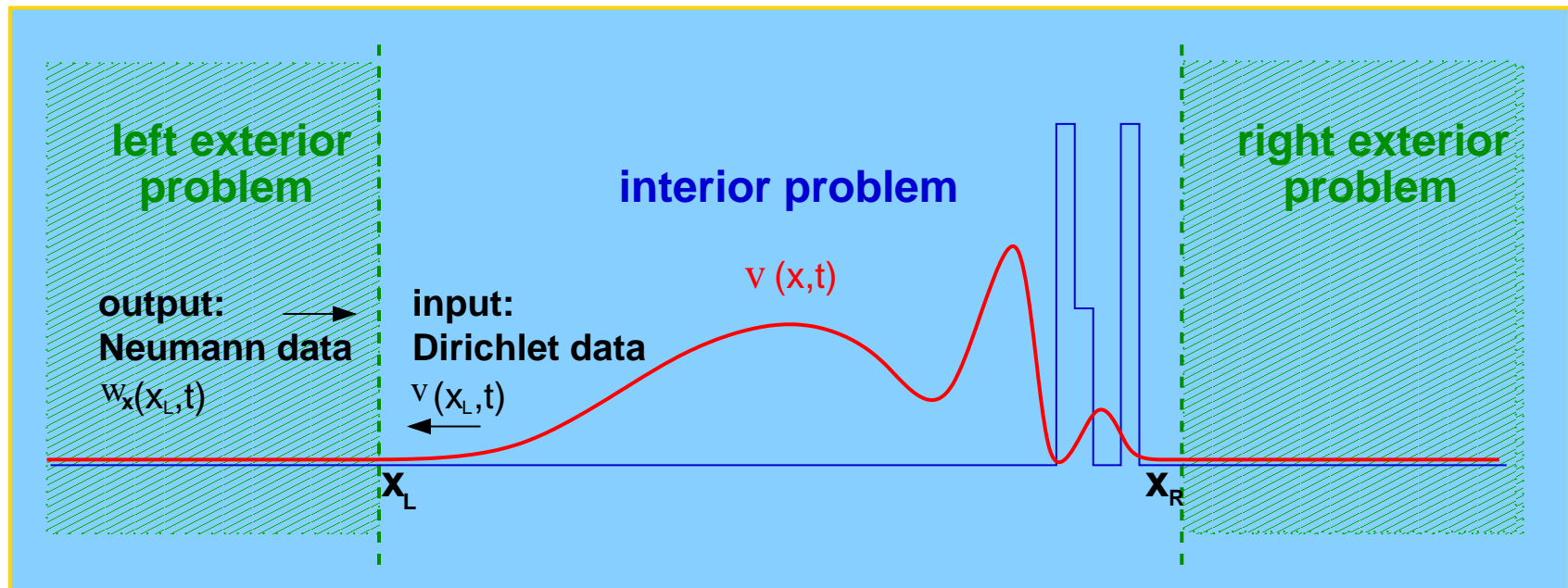
TBCs for the Schrödinger Equation

$$i\partial_t u = -\partial_x^2 u + V(x,t)u, \quad x \in \mathbb{R}, \quad t > 0$$

A1: $\text{supp } u(x, 0) \subseteq (x_l, x_r) \dots$ computational domain

A2: $V(x, t) = V_l, \quad x \leq x_l, \quad V(x, t) = V_r, \quad x \geq x_r$

(both assumptions can be relaxed significantly)



● **Goal:** reproduce $v = u|_{[x_l, x_r]}$ with **transparent BCs** at $x = x_l, x_r$

The Derivation of the right TBC

- right TBC $\partial_x u(x_r, t) = (T u)(x_r, t)$ from exterior problem:

$$i\partial_t w = -\partial_x^2 w + V_r w, \quad x > x_r$$

$$w(x, 0) = 0, \quad x > x_r$$

$$w(x_r, t) = v(x_r, t), \quad \text{decay condition } \lim_{x \rightarrow \infty} w(x, t) = 0$$

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- explicit solution of the right exterior problem by

Laplace transformation: $\hat{w}(x, s) = \int_0^\infty w(x, t)e^{-st} dt$

$$\partial_x^2 \hat{w} = (-is + V_r)\hat{w}, \quad x > x_r$$

solution: $\hat{w}(x, s) = A^+(s)e^{\sqrt{-is+V_r}x} + A^-(s)e^{-\sqrt{-is+V_r}x}$

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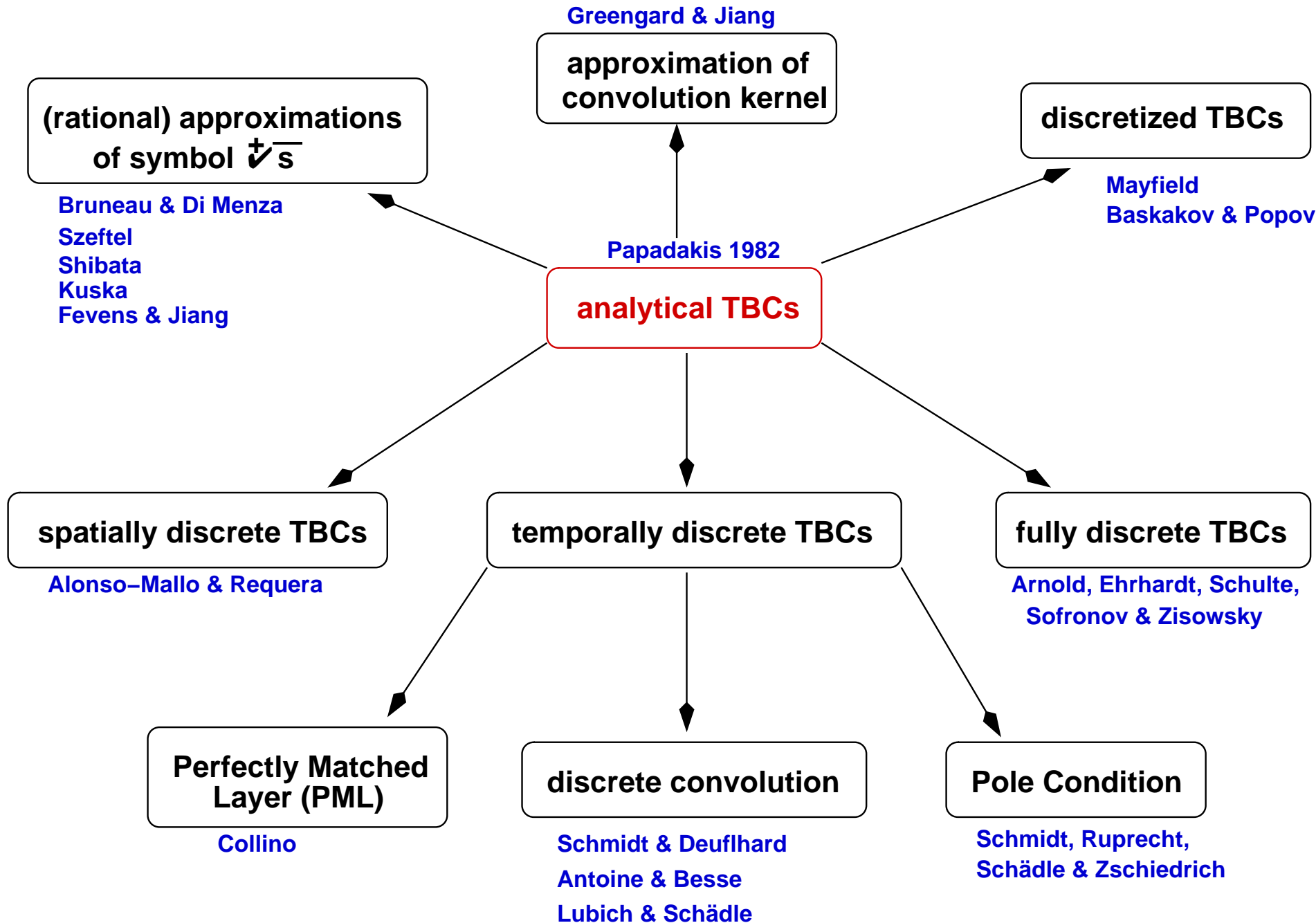
$$\partial_x^2 \hat{w} = (-is + V_r) \hat{w}, \quad x > x_r$$

solution must be in $L^2(\Omega)$: $\partial_x \hat{w}(x_r, s) = \hat{v}(x_r, s) e^{-\sqrt{-is+V_r}(x-x_r)}$

- inverse Laplace transformation \leadsto right TBC: [Papadakis '82]

$$\partial_x u(x_r, t) = -e^{-i\frac{\pi}{4}} \frac{1}{\sqrt{\pi}} e^{-iV_r t} \frac{d}{dt} \int_0^t \frac{u(x_r, \tau) e^{iV_r \tau}}{\sqrt{t-\tau}} d\tau$$

Approaches for transient Schrödinger Equation



Procedure to derive the analytic TBC

- (1) Split problem into coupled equations: interior and exterior problems
 - (2) Apply a Laplace transformation in time t
 - (3) Solve the ordinary differential equations in x
 - (4) Allow only ‘outgoing’ waves by taking decaying solution as $|x| \rightarrow \infty$
 - (5) Match Dirichlet and Neumann values at $x = x_l, x = x_r$
 - (6) Apply the inverse Laplace transformation to obtain the TBC
- For the IBVP on Ω with a DtN or a NtD TBC, existence and uniqueness of the solution has been proved, e.g. [Antoine/Besse’03]
 - Continuous TBCs fully solve the problem of confining the spatial domain to a bounded interval

but: their numerical discretization is not trivial at all!

here: two different approaches to derive (semi)discrete TBCs and ABCs

Temporally discrete TBCs

- SE discretized uniformly in time with A -stable multi-step method

$$\frac{i}{\Delta t} \sum_{j=0}^K \alpha_j u^{n-j} = \sum_{j=0}^K \beta_j (-\partial_x^2 + V) u^{n-j}, \quad n \geq K$$

- (2) instead of Laplace-transformation we apply a \mathcal{Z} -transformation

$$\mathcal{Z}(u^n) = \hat{u}(z) := \sum_{n=0}^{\infty} u^n z^{-n}, \quad z \in \mathbb{C}, \quad |z| > R(\mathcal{Z}(u^n))$$

- (3) 2nd order ODE $i \underbrace{\frac{\delta(z)}{\Delta t}}_{\leftrightarrow s} \hat{w}(z) = (-\partial_x^2 + V_r) \hat{w}(z), \quad x > x_r$

$$\delta(z) = \frac{\sum_{j=0}^K \alpha_j z^{K-j}}{\sum_{j=0}^K \beta_j z^{K-j}} \quad \text{generating function of time integration scheme}$$

- Assumption** on startup: $\text{supp}(u^j) \subset [x_l, x_r], \quad j = 0, 1, \dots, K - 1$

Example: trapezoidal rule discretization

$$i \frac{u^{n+1} - u^n}{\Delta t} = -\partial_x^2 \frac{u^{n+1} + u^n}{2} + \frac{V^{n+1}(x)u^{n+1} + V^n(x)u^n}{2}, \quad x \in \mathbb{R}$$

method (Crank-Nicolson) has generating function $\delta(z) = 2\frac{z-1}{z+1}$

(3) solving the ODE yields general solution

$$\hat{w}(x, z) = A^+(z) e^{i \sqrt{i \frac{\delta(z)}{\Delta t} - V_r} x} + A^-(z) e^{-i \sqrt{i \frac{\delta(z)}{\Delta t} - V_r} x}, \quad x > x_r$$

(4) $u^n \in L^2(]x_r, \infty[)$ \rightsquigarrow A^- must vanish

$$\mathcal{Z}(\partial_x w^n)(z) = i \sqrt{i \frac{\delta(z)}{\Delta t} - V_r} \mathcal{Z}(w^n)(z), \quad x = x_r$$

(6) inverse \mathcal{Z} -transformation \rightsquigarrow expression $\partial_x w^n(x_r)$ in terms of $w^k(x_r)$

$$(6) \partial_x v^{n+1} = \sum_{k=0}^{n+1} u_k v^{n+1-k} \text{ at } x = x_r \text{ with weights } u_n \text{ (for } V_r = 0)$$

Fully discrete TBCs

- SE discretized in space and time by Crank-Nicolson scheme

$$i \frac{u_j^{n+1} - u_j^n}{\Delta t} = -D_x^2 \frac{u_j^{n+1} + u_j^n}{2} + \frac{V_j^{n+1} u_j^{n+1} + V_j^n u_j^n}{2}, \quad j \in \mathbb{Z}$$

right artificial boundary is located at $x_r = x_l + J\Delta x$

- instead of Laplace-transformation we apply a \mathcal{Z} -transformation
- 2nd order difference equation with constant coefficients

$$\hat{w}_{j+1}(z) - 2 \left(1 - \frac{\Delta x^2}{2} \left(i \frac{\delta(z)}{\Delta t} + V_r \right) \right) \hat{w}_j(z) + \hat{w}_{j-1}(z) = 0, \quad j > J$$

- general solution

$$\hat{w}_j(z) = A^+(z) \chi^{j-J}(z) + A^-(z) \chi^{-(j-J)}(z), \quad j \geq J - 1$$

where $\chi(z)$ and $\chi(z)^{-1}$ are the roots of the quadratic equation

$$X^2 - 2 \left(1 - \frac{\Delta x^2}{2} \left(i \frac{\delta(z)}{\Delta t} + V_r \right) \right) X + 1 = 0$$

(4) decaying solutions $\hat{u}_j(z)$, $j \rightarrow \infty \rightsquigarrow$ choose **branch with $|\chi(z)| < 1$**

• \mathcal{Z} -transformed right discrete TBC [Arnold '95, Ehrhardt '01]

$$\hat{u}_{J-1}(z) = \chi(z)\hat{u}_J(z)$$

• transformed boundary kernel $\chi(z)$

$$\chi(z) = 1 - \frac{\Delta x^2}{2} \left(i \frac{\delta(z)}{\Delta t} - V_r \right) - \sqrt{\frac{\Delta x^2}{2} \left(i \frac{\delta(z)}{\Delta t} - V_r \right) \left(\frac{\Delta x^2}{2} \left(i \frac{\delta(z)}{\Delta t} - V_r \right) - 2 \right)}$$

(6) \mathcal{Z}^{-1} -transformation yields **convolution coefficients** for discrete TBC

$$(\chi_n) := \mathcal{Z}^{-1}(\chi(z)), \quad n \in \mathbb{N}_0$$

• right discrete TBC reads in physical space

$$u_{J-1}^n = \sum_{k=1}^n \chi_{n-k} u_J^k, \quad n \in \mathbb{N}$$

Discretizations and Approximations

- TBCs completely solve problem of confining unbounded domain (theoretically)
- for an (efficient) implementation the TBCs have to be discretized and/or approximated
- three main approaches in the literature
 - discretizations of the TBC by quadrature rules
 - approximation of convolution kernel by sums of exponentials
 - rational approximations of Fourier-symbol of convolution kernel

Discretizations by quadrature formulas

- first idea to incorporate TBC in scheme is an ad-hoc discretization

$$\begin{aligned} & \int_0^{t_{n+1}} \frac{u_x(x_r, t_{n+1} - \tau) e^{-iV_r\tau}}{\sqrt{\tau}} d\tau \\ & \approx \frac{1}{\Delta x} \sum_{k=0}^n (u_J^{n+1-k} - u_{J-1}^{n+1-k}) e^{-iV_r k \Delta t} \int_{t_k}^{t_{k+1}} \frac{d\tau}{\sqrt{\tau}} \\ & = \frac{2\sqrt{\Delta t}}{\Delta x} \sum_{k=0}^n \frac{(u_J^{n+1-k} - u_{J-1}^{n+1-k}) e^{-iV_r k \Delta t}}{\sqrt{k+1} + \sqrt{k}} \end{aligned}$$

Discretizations by quadrature formulas

- first idea to incorporate TBC in scheme is an ad-hoc discretization

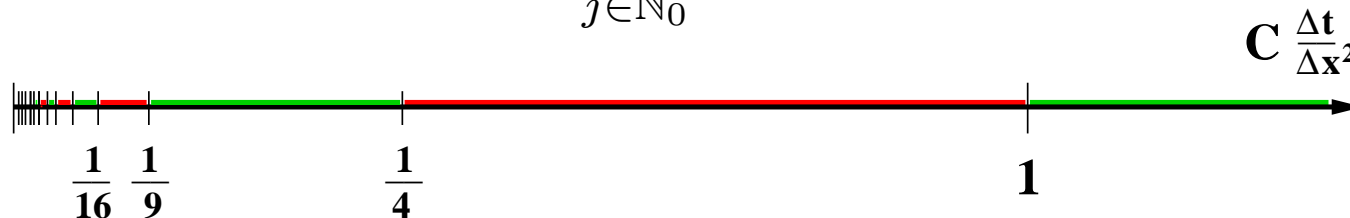
↪ discretized TBC for the SE

$$u_J^{n+1} - u_{J-1}^{n+1} = \frac{\Delta x}{2B\sqrt{\Delta t}} u_J^{n+1} - \sum_{k=1}^n (u_J^{n+1-k} - u_{J-1}^{n+1-k}) \tilde{\ell}_k$$

with $B = -\frac{1}{\sqrt{2\pi}} e^{i\frac{\pi}{4}}, \quad \tilde{\ell}_k = \frac{e^{-iV_r k\Delta t}}{\sqrt{k+1} + \sqrt{k}}$

- **Theorem** [Mayfield '89]: CN-FD scheme for the Schrödinger equation with a certain discretized analytic TBCs is **stable** \iff

$$\frac{4}{\pi} \frac{\Delta t}{\Delta x^2} \in \bigcup_{j \in \mathbb{N}_0} [(2j+1)^{-2}, (2j)^{-2}]$$



Rational approximations of the Fourier symbol

- In pseudodifferential calculus the Laplace transform of the kernel $\sqrt[+]{s}$ is identified with the Fourier symbol $\sqrt[+]{i\omega}$
- now: rational approximations of Fourier symbol of convolution kernel
- fractional derivative operator $\partial_t^{1/2}$ in analytic TBC is **nonlocal-in-time** (due to the non-polynomial nature of its Fourier symbol $\sqrt[+]{i\omega}$)

- **Example:** In the **spatial discrete case** the Fourier symbol is given in

$$\chi(s) = 1 - \frac{\Delta x^2}{2}(is - V_r) + \sqrt[+]{\frac{\Delta x^2}{2}(is - V_r)\left(\frac{\Delta x^2}{2}(is - V_r) - 2\right)}$$

- rational approximation of these symbols allows for a **local-in-time** approximated convolution
- For all of the subsequent methods some **a-priori information** on the dominant wavenumber of the solution at the boundary is needed

Bruneau–Di Menza, Szeftel, Shibata, and Kuska

- right analytic TBC in Fourier space ($V_r = 0$)

$$\partial_x \hat{u}(x_r, \omega) = -e^{i\pi/4} \sqrt[4]{i\omega} \hat{u}(x_r, \omega)$$

- approximate the symbol $\sqrt[4]{i\omega}$ by a rational function

$$R_m(i\omega) = \sum_{k=0}^m a_k^m - \sum_{k=1}^m \frac{a_k^m d_k^m}{i\omega + d_k^m}, \quad a_k^m, d_k^m > 0$$

Bruneau–DiMenza require $R_m(i\omega)$ to interpolate $\sqrt[4]{i\omega}$ at $2m + 1$ distinct points

Szeftel also uses a rational approximation of $\sqrt[4]{i\omega}$, but different coefficients:

- Padé approximation
- coefficients by minimizing the reflection coefficient

Shibata linear approximation with two intersection points

Kuska 1/1–Padé approximation about dominant frequency ω_0 to choose

Approach of Fevens and Jiang

- family of absorbing boundary conditions (ABCs) of order p

$$\prod_{l=1}^p \left(i \frac{\partial}{\partial x} + a_l \right) u = 0, \quad p \in \mathbb{N}$$

- from the shape $u = e^{i(kx - \omega t)}$ of a **plane wave** one sees:
all waves with wavenumber $k = a_l$ are perfectly absorbed
- **well-posedness** for this class of (analytic) ABCs was established
- with **low order choices** $p = 2$ or $p = 3$; $a_1 = a_2 = a_3$ one recovers the ABCs of Shibata and of Kuska

Numerical Example

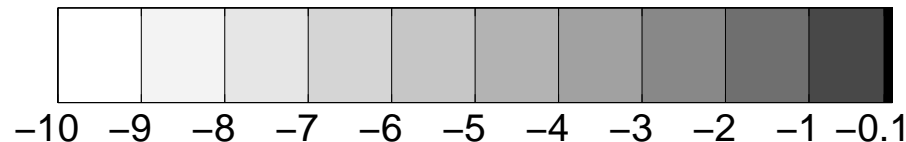
- SE with a vanishing potential $V \equiv 0$ and a Gaussian initial condition

$$u^I(x) = \exp(-x^2 + ik_0x), \quad x \in \mathbb{R}$$

- analytic solution can be calculated explicitly

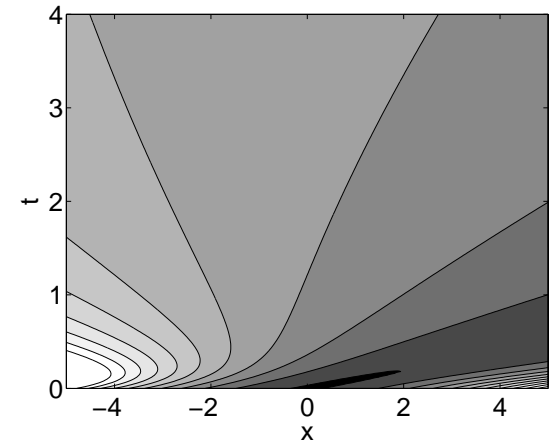
$$u_{\text{ex}}(x, t) = \sqrt{\frac{i}{-4t + i}} \exp\left(\frac{-ix^2 - k_0x + k_0^2t}{-4t + i}\right), \quad x \in \mathbb{R}, t > 0$$

- comput. domain $\Omega_{\text{int}} =] - 5, 5[$, frequency $k_0 = 8$, final time $T_f = 4$
- high frequency of solution needs a very good approximation of $\partial_t^{1/2}$
- $J = 40000$ grid points in spatial direction and time step $\Delta t = 10^{-4}$
- contour of $\log_{10}(|u|)$ to show small level of reflections
(numerical reflections cannot be visualized in traditional contour plot)

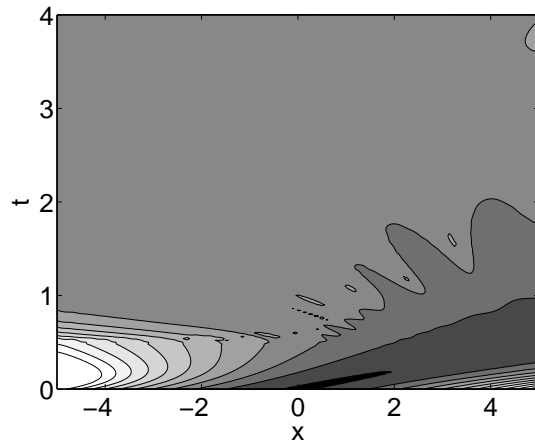


Example: Fevens–Jiang family

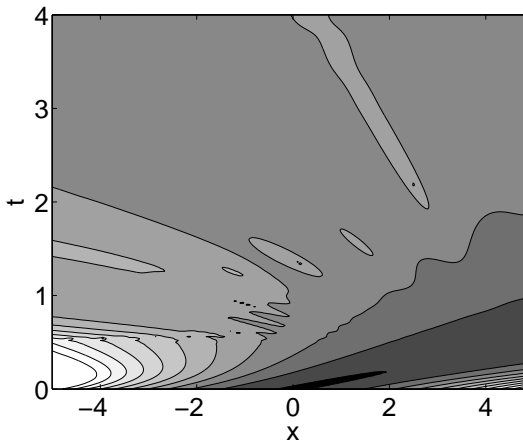
- Figure (a) contour plot of the solution for the fully discrete scheme
- By construction there are no reflections at all from the discrete TBC, so it serves as a reference for the other methods



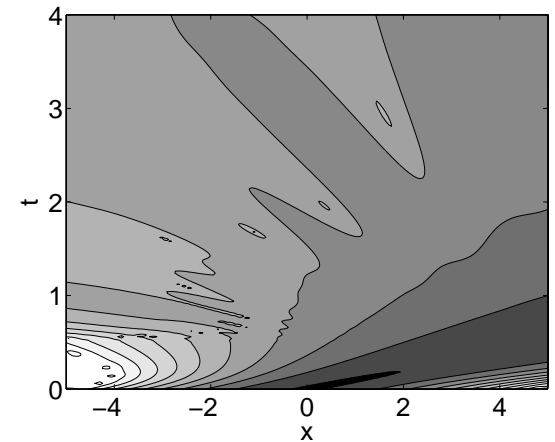
() Arnold–Ehrhardt



() Shibata



() Kuska

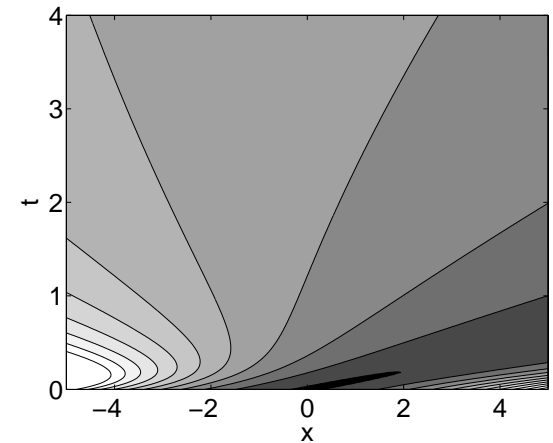


() Fevens

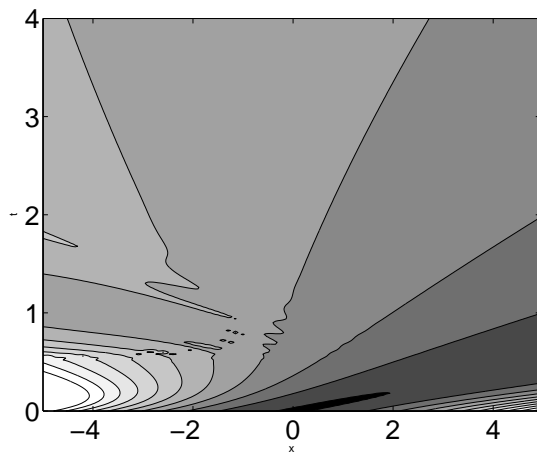
- a levels increase improves significantly the solution
- these older methods are less competitive

Example: Approximation of the square root

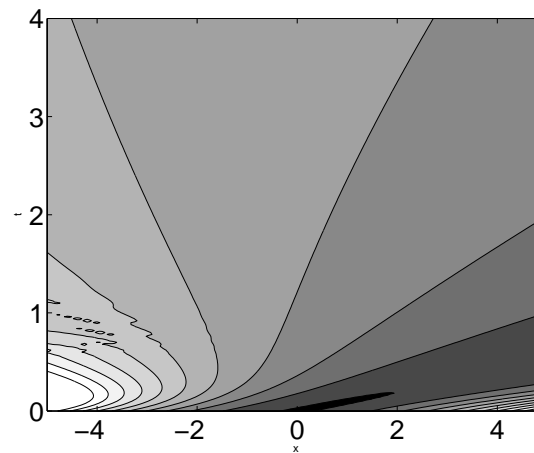
- Figure (e) again as reference solution
- method (f) needs 27 coefficients
- method (g) uses 20 Padé coefficients
- method (h) only uses 3 coefficients
(minimization of reflection coefficient)



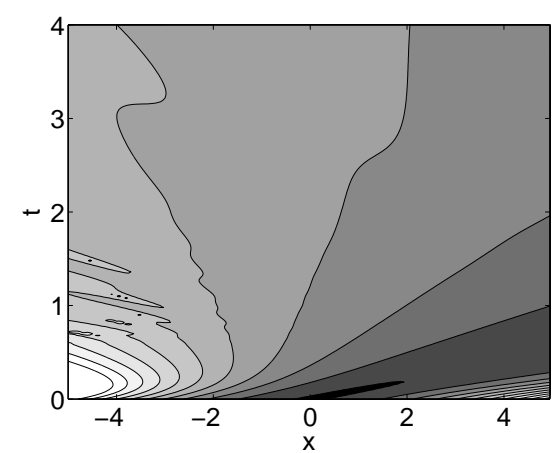
(e) Arnold–Ehrhardt



(f) Di Menza



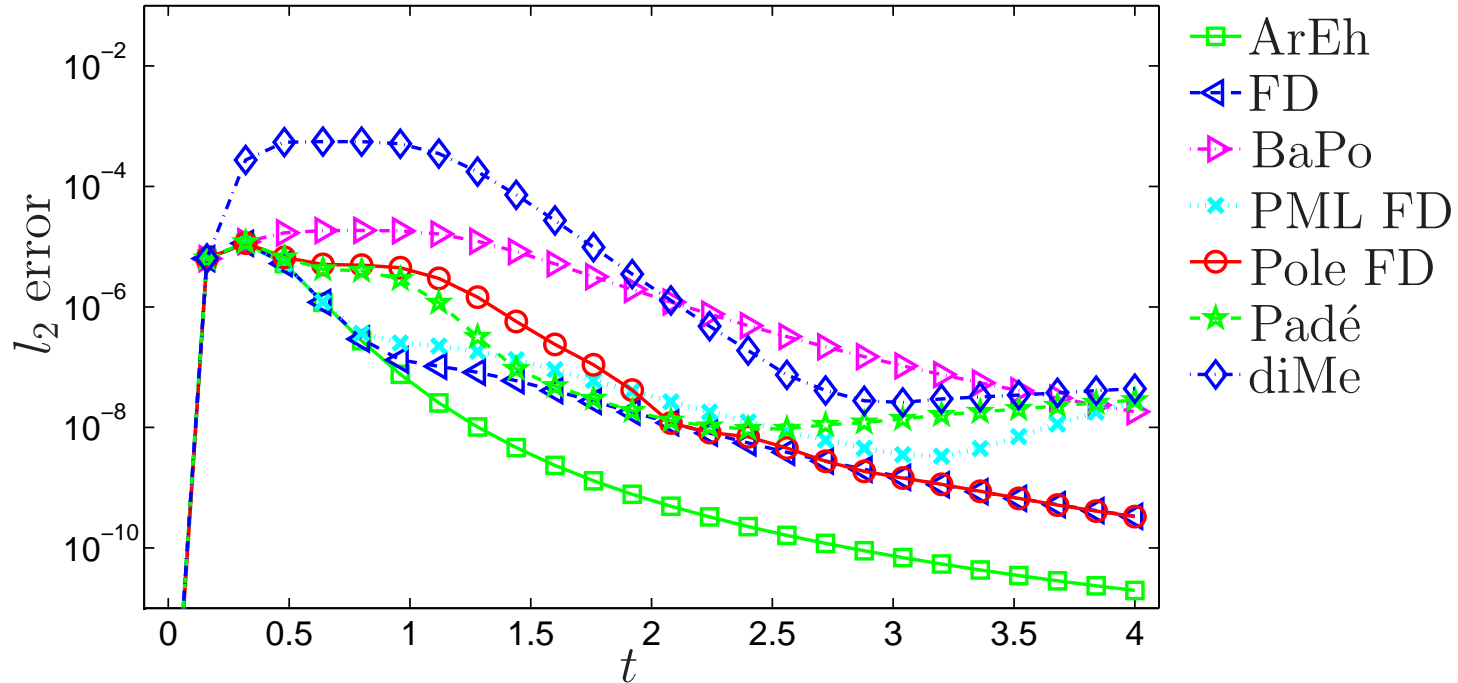
(g) Padé



(h) Szeftel

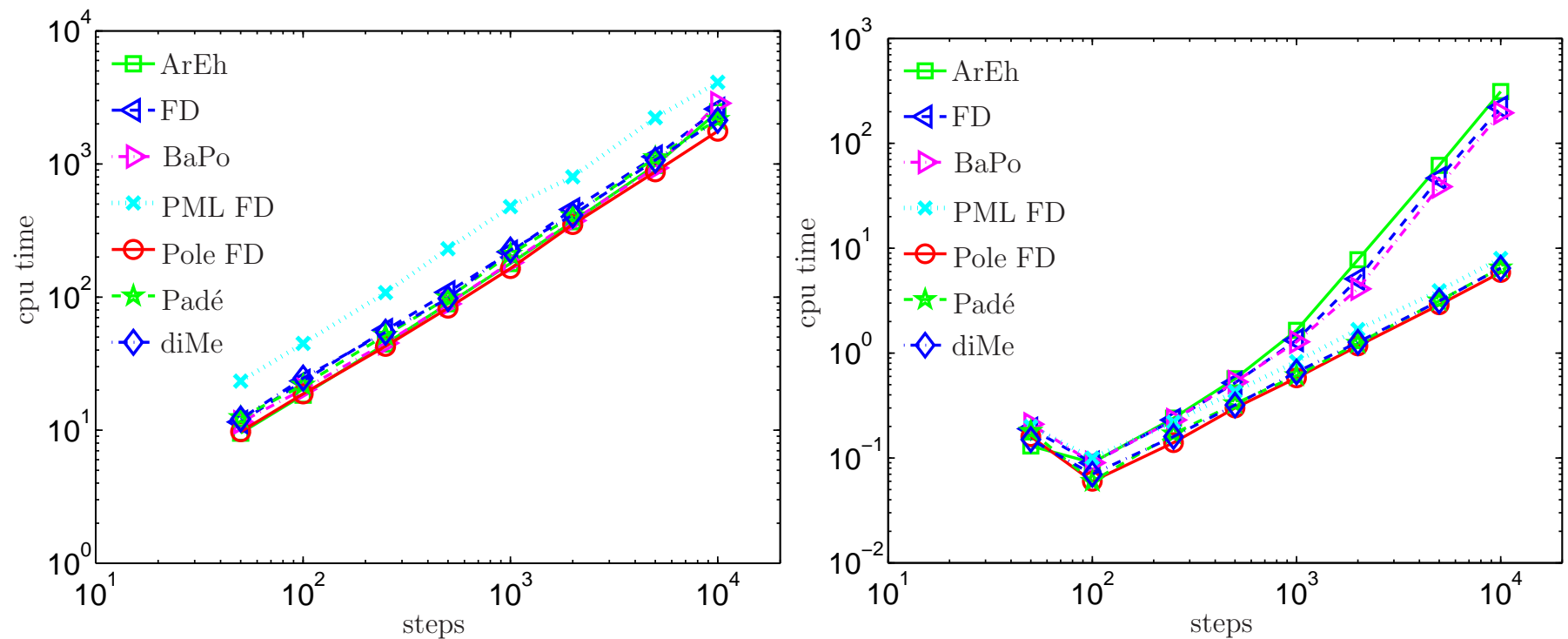
- solutions built with a square root approximation are far better

Example: first group of methods



- Time evolution of the spatial l_2 error for various finite difference methods and the fixed step sizes $\Delta x = 2.5 \cdot 10^{-4}$, $\Delta t = 10^{-4}$
- method by Di Menza (**diMe**) shows **strong reflection** producing an error about 10^2 times larger than the interior discretization error
- method of Baskakov–Popov (**BaPo**) induces a **reflection** that is about the same magnitude as the interior discretization error

Example: cpu time as function of number of steps



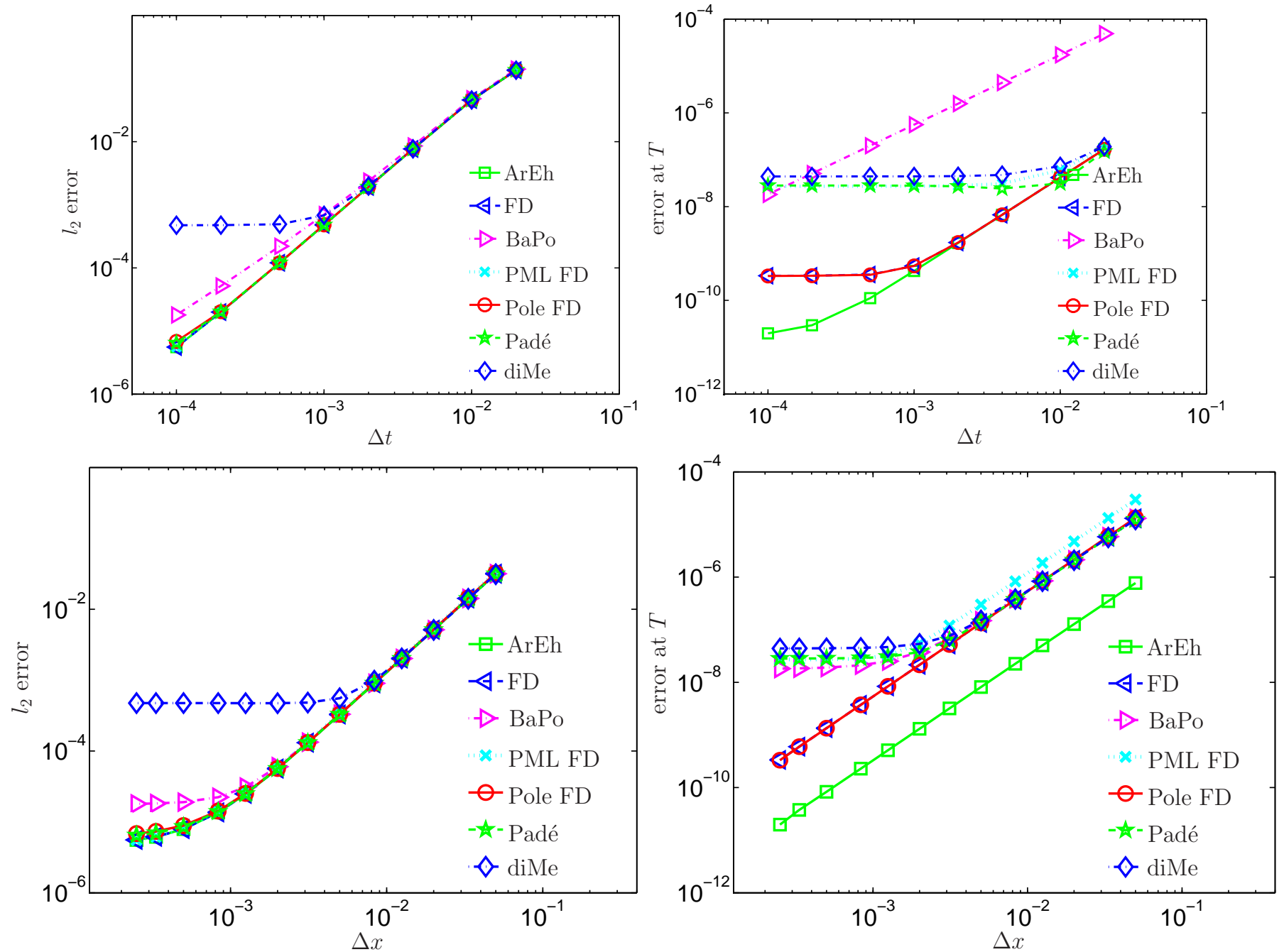
● **left figure: fine spatial mesh** (#unknowns 40.000)

- solution of the linear system is **most time consuming part**
⇒ the different methods can hardly be distinguished

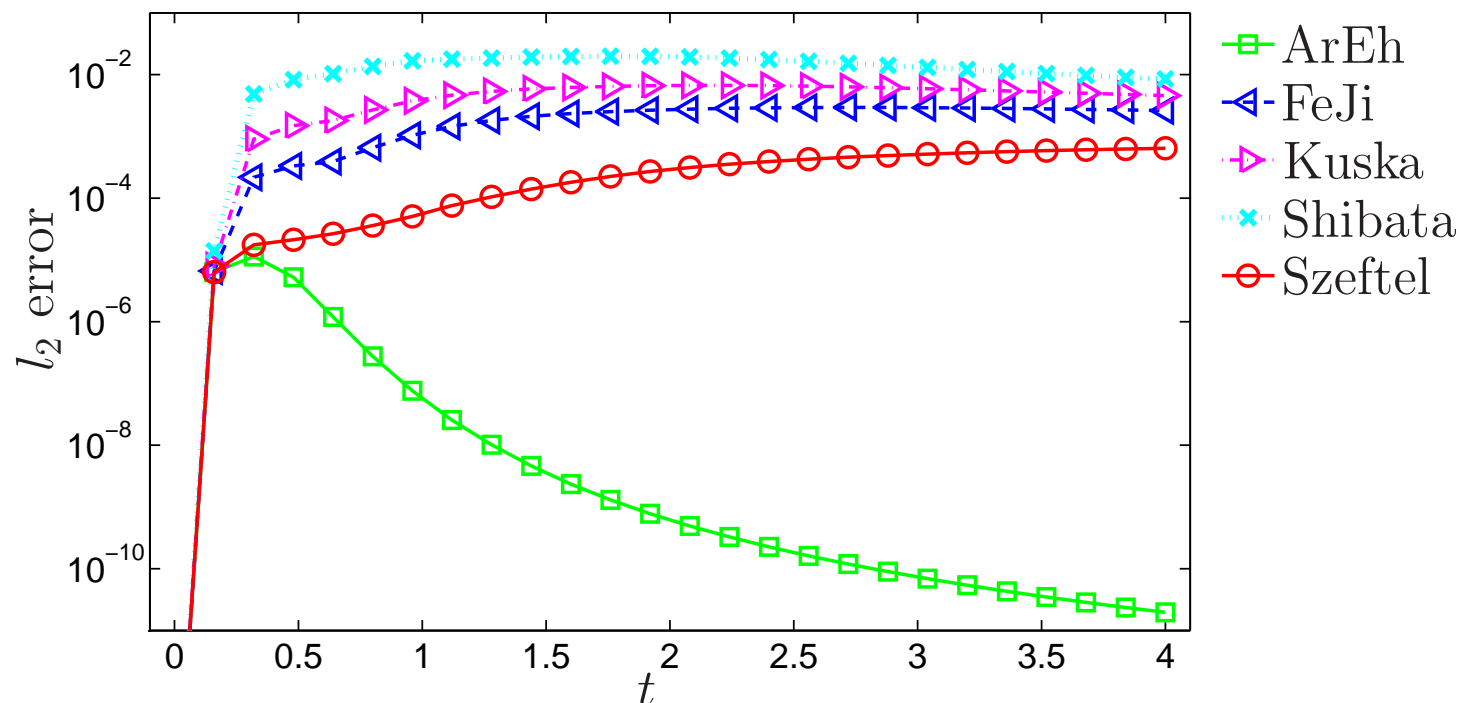
● **right figure: coarse spatial mesh** (about 200 unknowns)

- **ArEh, FD and BaPo** methods do not scale linearly
quadratic operation count of the convolution starts to dominate

Example: convergence of the methods

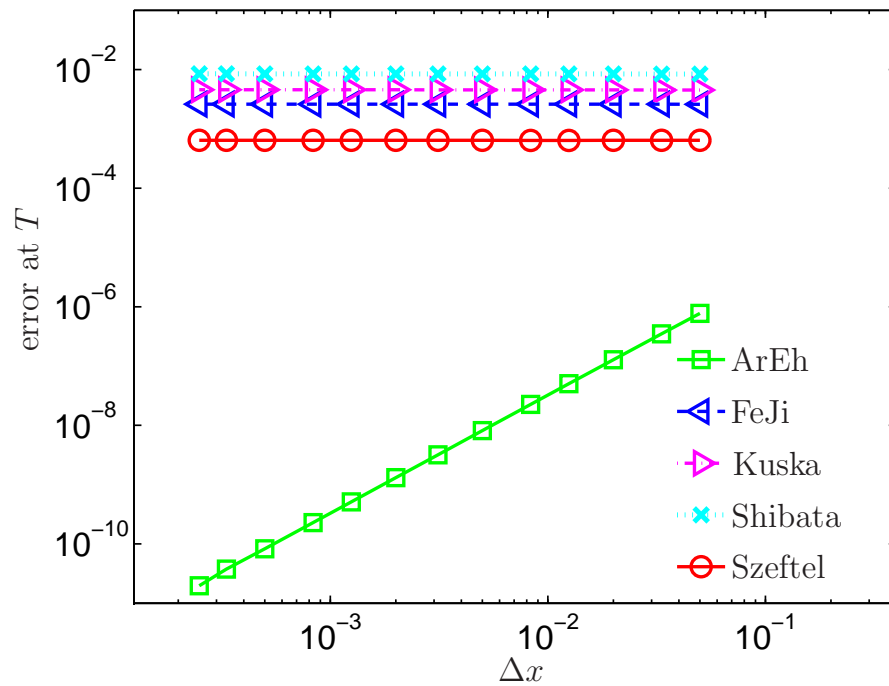
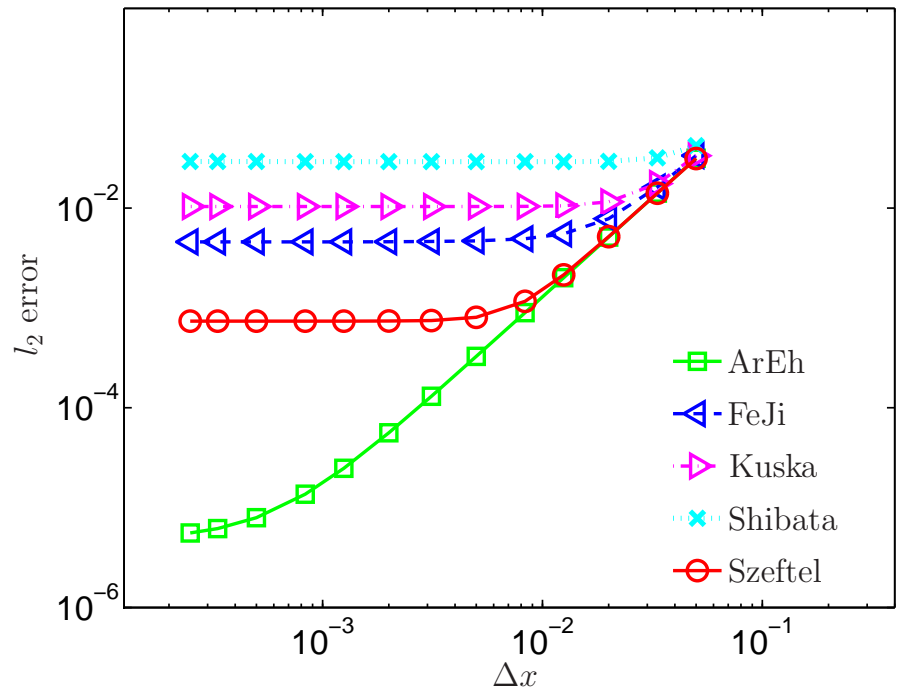
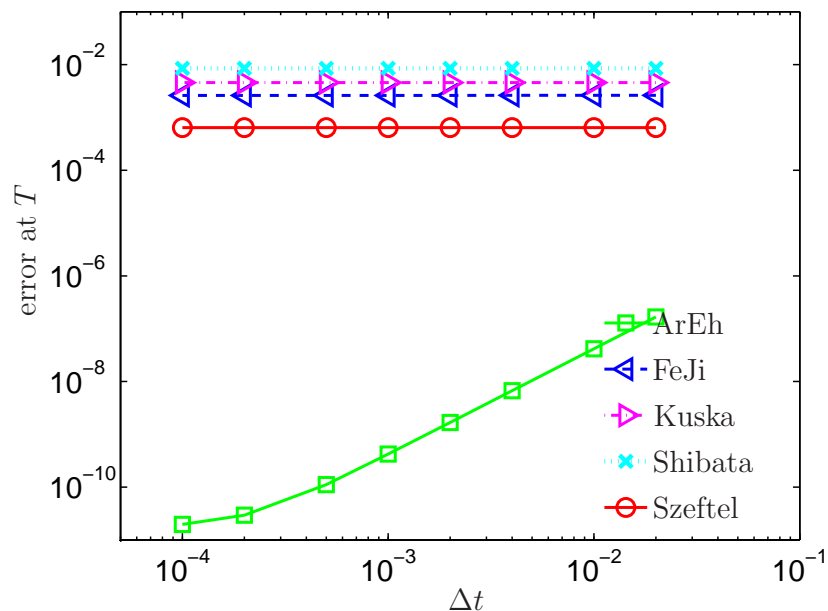
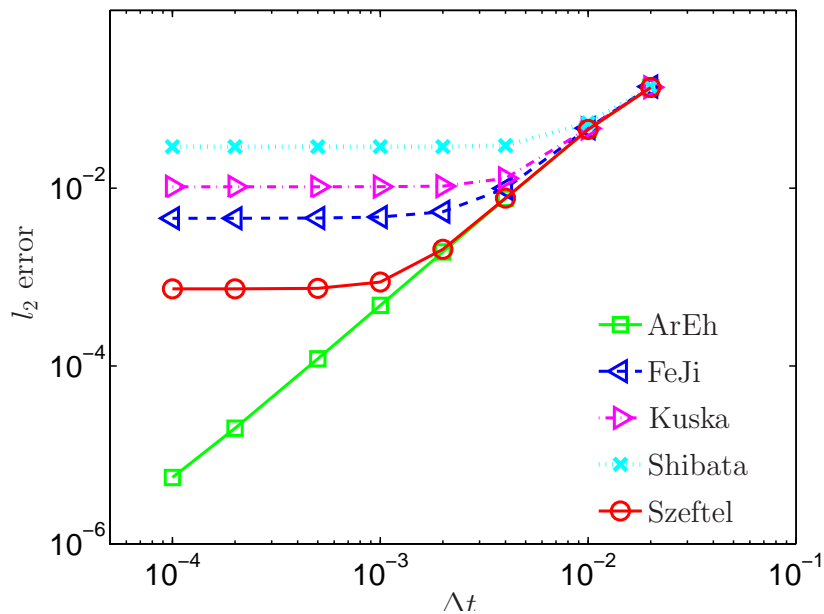


Example: second group of methods

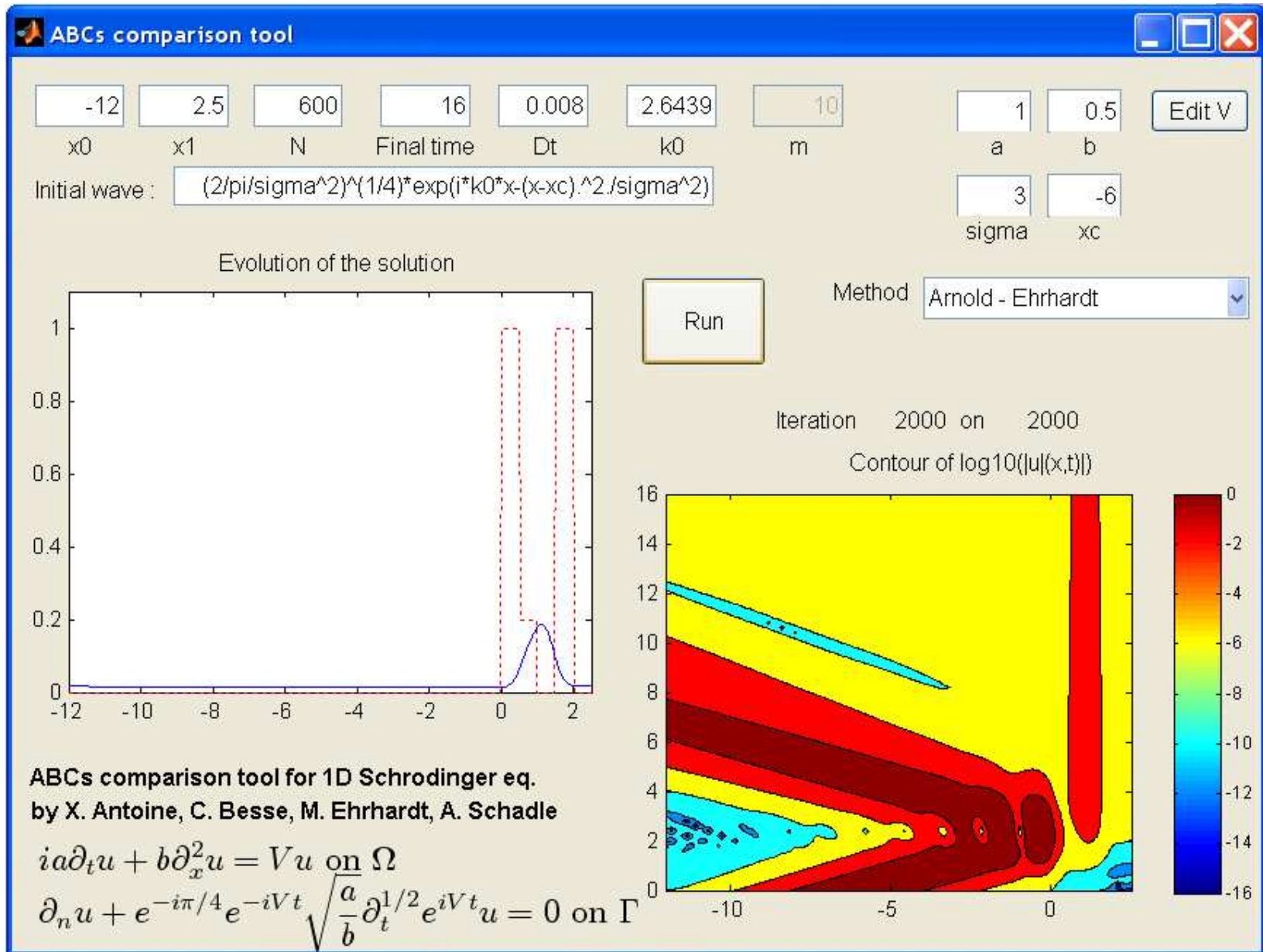


- Time evolution of the spatial l_2 error for various finite difference methods and the fixed step sizes $\Delta x = 2.5 \cdot 10^{-4}$, $\Delta t = 10^{-4}$
- methods of the Fevens–Jiang family **FeJi**, Kuska and Shibata all show **strong reflections**
- method by Szeftel performs better (uses only 3 coefficients!)

Example: convergence of the methods



Comparison tool for 1D Schrödinger equation



ABCs for Nonlinear Schrödinger Equations

new field [Szeftel '05], [Antoine, Besse & Descombes '05], [Zheng '05]

- Schrödinger equation $iu_t + u_{xx} + f(|u|^2)u = 0$ (NLS)
e.g. the cubic Schrödinger equation ($f = \lambda|u|^2$)
- linear TBCs work well for reaction–diffusion eqs. but not for NLS
- **Problem:** integral transformation methods for (discrete) TBCs for linear equations **do not work** for nonlinear problems!

ABCs for Nonlinear Schrödinger Equations

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- linear TBCs work well for reaction–diffusion eqs. but not for NLS
- **Problem:** integral transformation methods for (discrete) TBCs for linear equations **do not work** for nonlinear problems!
- **Idea:** transform NLS into a linear equation (with variable coefficients)
 - potential strategy
 - phase function approach
 - parilinearization

apply strategy of [Engquist & Majda '79] (adapted for Schrödinger eq.)
and backtransform the obtained ABC

The Potential Strategy

We consider the cubic nonlinear Schrödinger equation

$$\begin{cases} iu_t + u_{xx} + \lambda|u|^2u = 0, & x \in \mathbb{R}, \quad t > 0 \\ u(x, 0) = u^I(x), & x \in \mathbb{R} \end{cases}$$

- Nonlinearity = potential multiplied by the unknown function u
 \rightsquigarrow linear Schrödinger equation with a potential $V(x, t) = \lambda|u(x, t)|^2$
- Method of [Engquist & Majda '79] \rightsquigarrow second order absorbing BC

$$u_x + e^{-i\pi/4} \partial_t^{1/2} u - \frac{V}{2} e^{i\pi/4} I_t^{1/2} u = 0, \quad x = 0 \quad (\text{ABC2})$$

- Recalling $V = \lambda|u|^2$ (ABC2) becomes

$$u_x + e^{-i\pi/4} \partial_t^{1/2} u - \lambda \frac{|u|^2}{2} e^{i\pi/4} I_t^{1/2} u = 0, \quad x = 0$$

$$\partial_t^{1/2} \varphi(t) = \frac{1}{\sqrt{\pi}} \partial_t \int_0^t \frac{\varphi(\tau)}{\sqrt{t-\tau}} d\tau, \quad I_t^{1/2} \varphi(t) = \frac{1}{\sqrt{\pi}} \int_0^t \frac{\varphi(\tau)}{\sqrt{t-\tau}} d\tau$$

The Phase Function Transformation Strategy

We consider the cubic nonlinear Schrödinger equation

$$\begin{cases} iu_t + u_{xx} + \lambda|u|^2u = 0, & x \in \mathbb{R}, \quad t > 0 \\ u(x, 0) = u^I(x), & x \in \mathbb{R} \end{cases}$$

- introduce phase function $\mathcal{V}(x, t) = \lambda \int_0^t |u(x, \tau)|^2 d\tau$
- new unknown function $v(x, t) = e^{i\mathcal{V}(x, t)}u(x, t)$ satisfies

$$\begin{cases} iv_t + v_{xx} + 2i\mathcal{V}_x v_x + (i\mathcal{V}_x x - (\mathcal{V}_x)^2)v = 0, & x \in \mathbb{R}, \quad t > 0 \\ v(x, 0) = u^I(x), & x \in \mathbb{R} \end{cases}$$

↪ linear variable coefficients Schrödinger equation

- Method of [Engquist & Majda '79] ↪ second order absorbing BC

$$u_x + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} (e^{-i\mathcal{V}} u) + i \frac{V_x}{4} e^{i\mathcal{V}} I_t^{1/2} (e^{-i\mathcal{V}} u) = 0, \quad x = 0$$

asymptotic ABCs by Leibnitz derivation rule for fractional operators

Conclusions

We have presented several different techniques to solve numerically the time–dependent SE on unbounded domains

- **comparison of several implementations** of the classical TBC and ABCs into finite difference (and finite element discretizations)
- mainly the one–dimensional case but also the **cubic nonlinear case** (for the **2D case** cf. the review paper or the recent work Arnold, E., Schulte & Sofronov, Preprint No. 41–2007, TU Berlin)
- **several numerical examples** comparing the proposed boundary conditions w.r.t. different kind of errors and the cpu time
- freely available **graphical user interface** (written in MATLAB) covering most of the presented approaches
- **review paper / software:** <http://www.tbc-review.de.vu>

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- **Future:** most numerical schemes for NLS are of split–step type and discrete TBCs for split-step schemes are already derived numerical tests (**discrete potential strategy**) indicates that discrete ABCs are (at least) competitive Zisowsky & E., Preprint No. 11–2007, TU Berlin, (accepted: Math. Comput. Modelling)

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Thank You for Your Attention!