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

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

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Artificial Boundary Conditions for linear and nonlinear Schrödinger equations

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Outline

- Numerical Computation on unbounded Domains
- Transparent BCs for 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)

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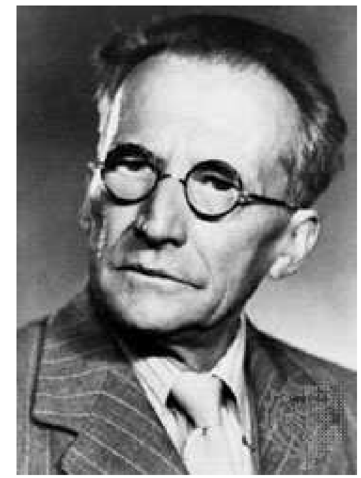
- **Numerical computation**: one has to restrict the computational domain Ω by artificial boundary conditions or absorbing layers
- If approximate solution coincides on Ω with exact solution, these BCs are called transparent boundary conditions (TBCs)
- Constructed artificial boundary conditions should
  - 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

The Schrödinger Equation

- SE is the fundamental equation of quantum mechanics developed 1926 by Austrian physicist Erwin Schrödinger
- describes form of probability waves that govern motion of small particles

  specifies how these waves are altered by external influences



(1887–1961)

- it is called Fresnel's equation in optics and 'parabolic equation' in acoustics & geophysics

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

$u(x,t) \in \mathbb{C}$ wave function, $V(x,t) \in \mathbb{R}$ given potential

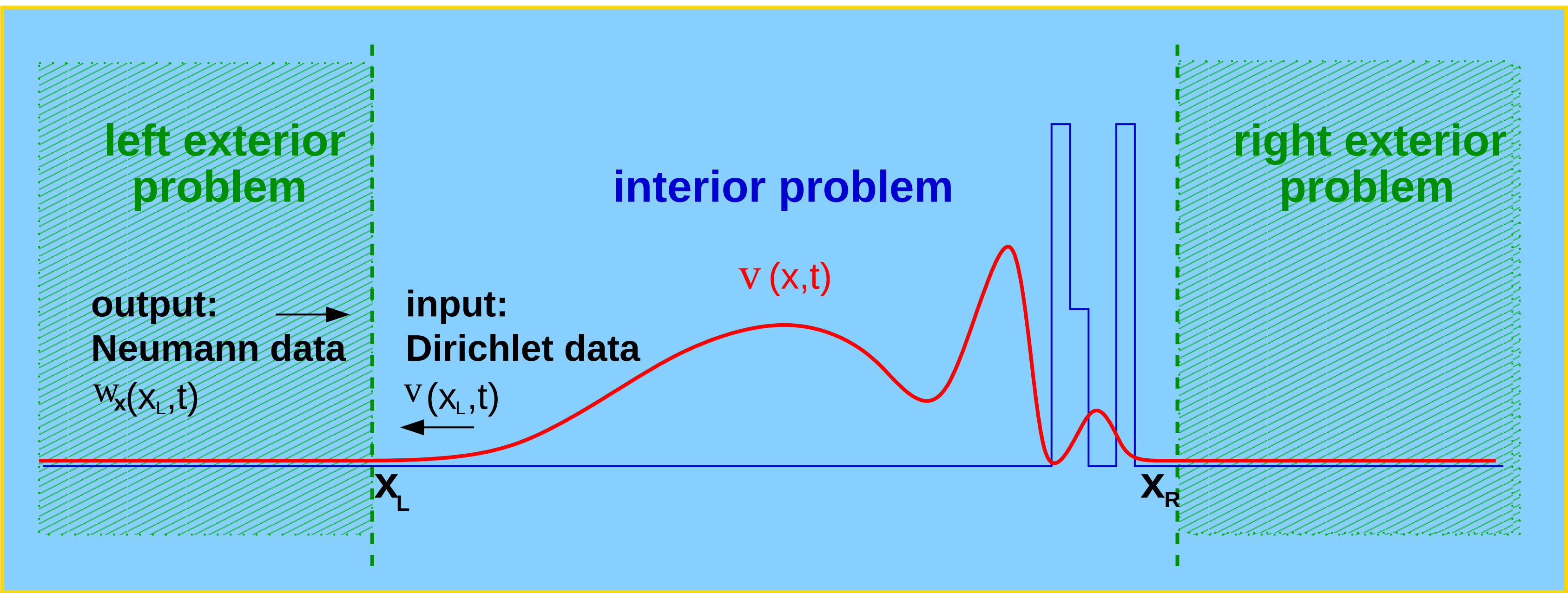
TBCs for the Schrödinger Equation

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

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

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

(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:

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

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

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

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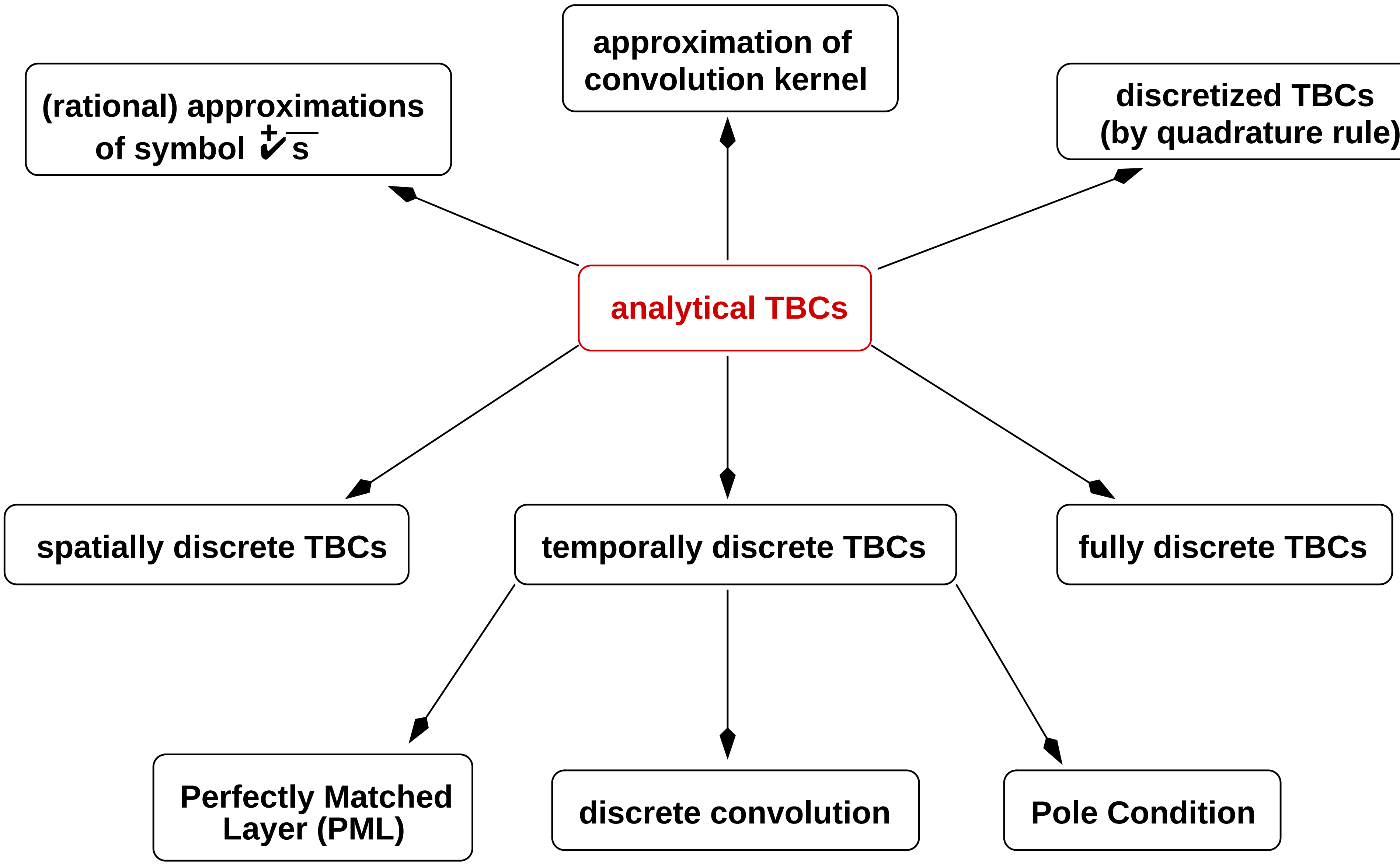
solution must be in $L^2(\Omega)$: $\partial_x \hat{w}(x_r,s) = \hat{v}(x_r,s)\,e^{-\sqrt[+]{-is+V_r}\,(x-x_r)}$

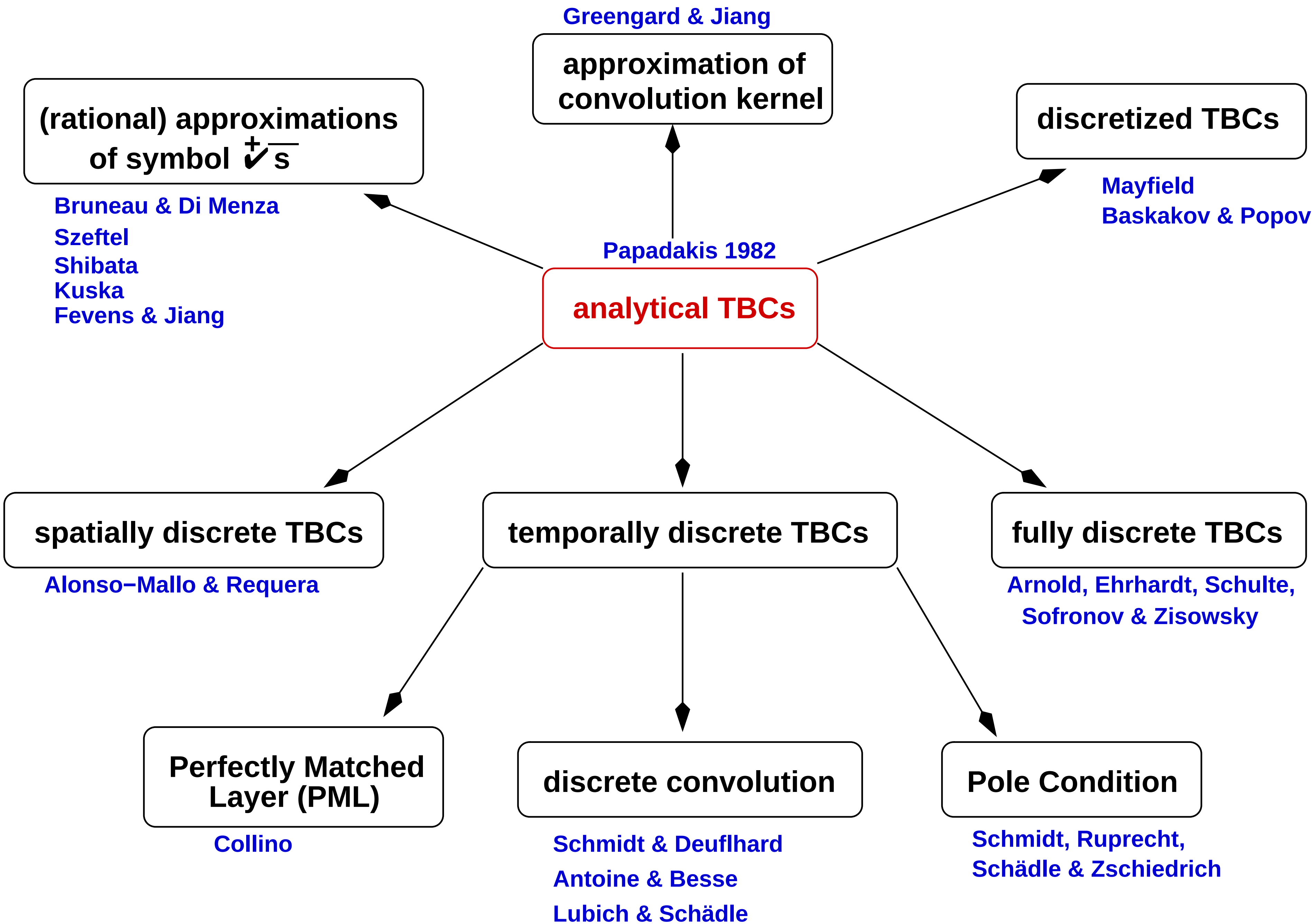
- inverse Laplace transformation $\rightsquigarrow$ right TBC: [Papadakis '82]

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

Approaches for transient Schrödinger Equation



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 $|x| \to \infty$

(5) Match Dirichlet and Neumann values at $x = x_l$, $x = x_r$

(6) Apply the inverse Laplace transformation to obtain the TBC

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- 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

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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

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

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

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

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

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

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

Example: trapezoidal rule discretization

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

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

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

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

$$u_k = -e^{-\frac{i\pi}{4}} \frac{\sqrt{2}}{\sqrt{\Delta t}} (-1)^k \tilde{u}_k, \quad k \in \mathbb{N}_0,$$

$$(\tilde{u}_0\, \tilde{u}_1, \tilde{u}_2, \tilde{u}_3, \tilde{u}_4, \tilde{u}_5, \dots) = \left(1, 1, \frac{1}{2}, \frac{1}{2}, \frac{1\cdot 3}{2\cdot 4}, \frac{1\cdot 3}{2\cdot 4}, \dots\right)$$

Fully discrete TBCs

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

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

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

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

(3) 2nd order difference equation with constant coefficients

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

- 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 $\hat{u}_j(z)$, $j \to \infty$ $\leadsto$ choose branch with $|\chi(z)| < 1$

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

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

- 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

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

- right discrete TBC reads in physical space

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

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

$$\int_0^{t_{n+1}} \frac{u_x(x_r, t_{n+1}-\tau)\, e^{-iV_r\tau}}{\sqrt{\tau}}\, d\tau$$

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

$$= \frac{2\sqrt{\Delta t}}{\Delta x} \sum_{k=0}^{n} \frac{(u_J^{n+1-k} - u_{J-1}^{n+1-k})\, e^{-iV_r k\Delta t}}{\sqrt{k+1}+\sqrt{k}}$$

Discretizations by quadrature formulas

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

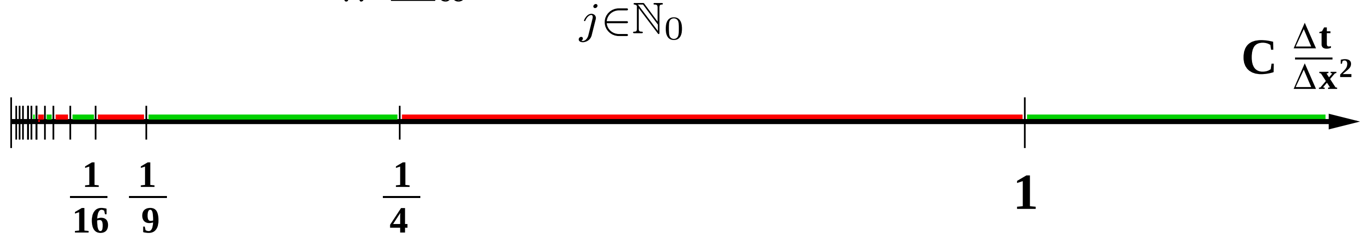
$\rightsquigarrow$ discretized TBC for the SE

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

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

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

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



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 ($V_r = 0$)

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

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

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

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

Szeftel also uses a rational approximation of $\sqrt[+]{i\omega}$, 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

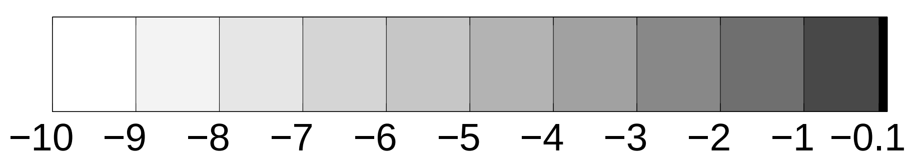
- SE with a vanishing potential $V \equiv 0$ and a Gaussian initial condition

$$u^I(x) = \exp(-x^2 + ik_0 x), \quad x \in \mathbb{R}$$

  - analytic solution can be calculated explicitly

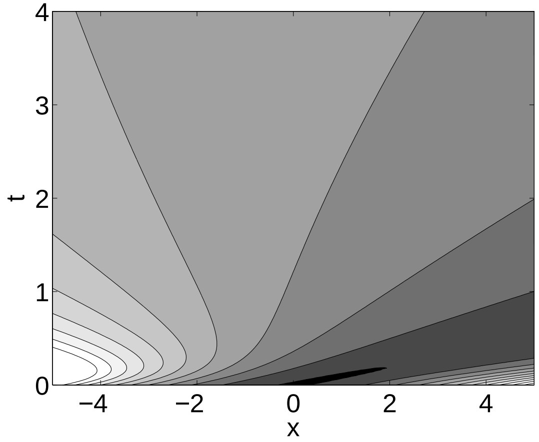
$$u_{\text{ex}}(x,t) = \sqrt{\frac{i}{-4t+i}} \exp\left(\frac{-ix^2 - k_0 x + k_0^2 t}{-4t+i}\right), \quad x \in \mathbb{R},\ t > 0$$

- comput. domain $\Omega_{int} =]-5,5[$, 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)

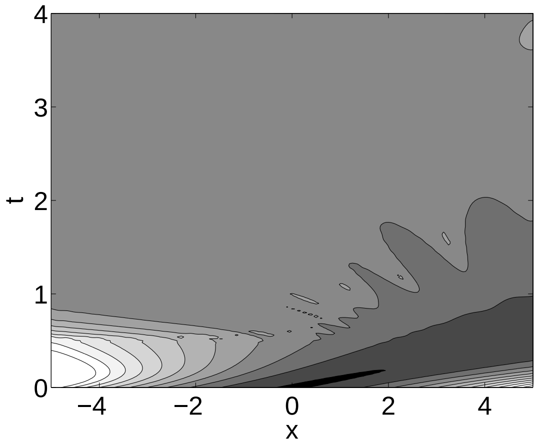


Example: Fevens–Jiang family

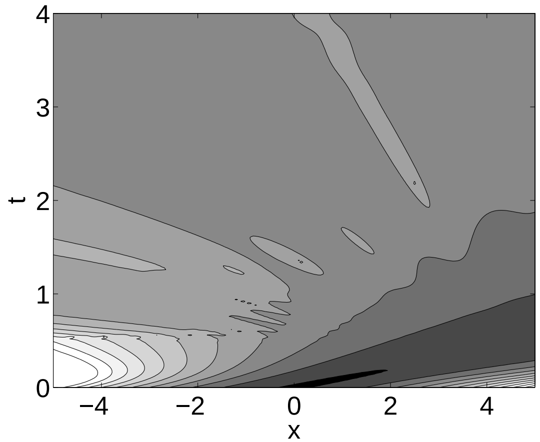
- Figure (a) contour plot of the solution for the fully discrete scheme
- By construction there are no reflections at all from the discrete TBC, so it serves as a reference for the other methods



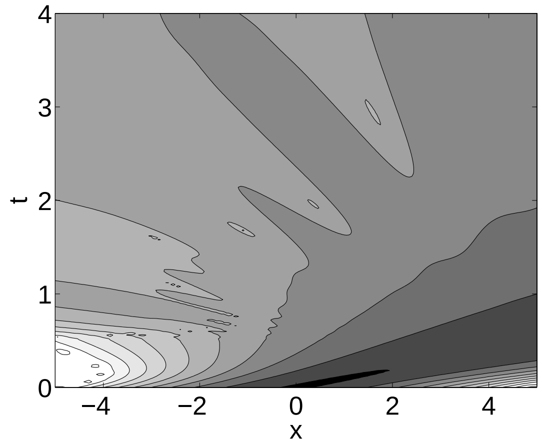
(a) Arnold–Ehrhardt



(b) Shibata



(c) Kuska

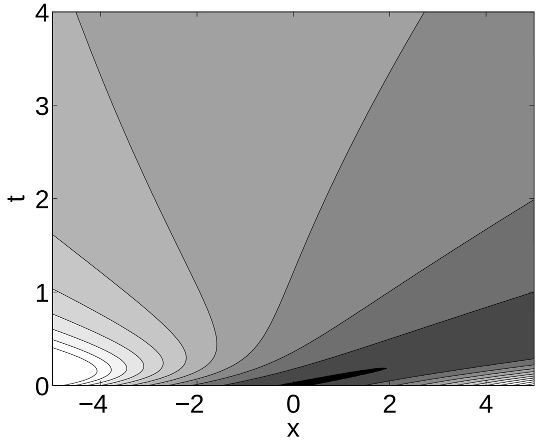


(d) Fevens

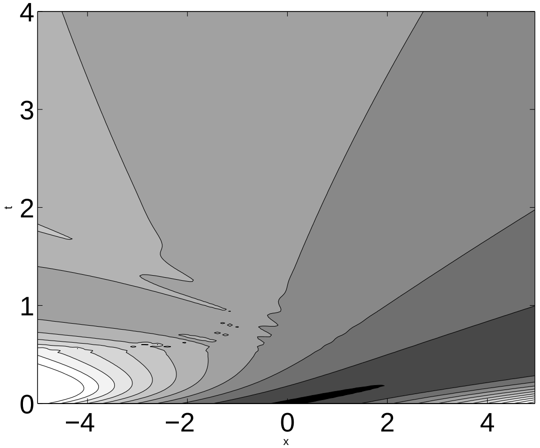
- a levels increase improves significantly the solution
- these older methods are less competitive

Example: Approximation of the square root

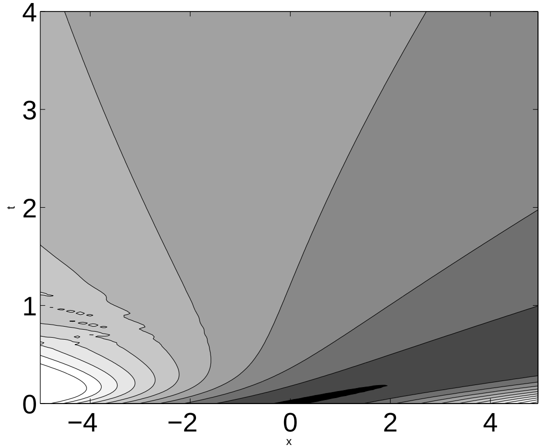
- Figure (e) again as reference solution
- method (f) needs 27 coefficients
- method (g) uses 20 Padé coefficients
- method (h) only uses 3 coefficients (minimization of reflection coefficient)



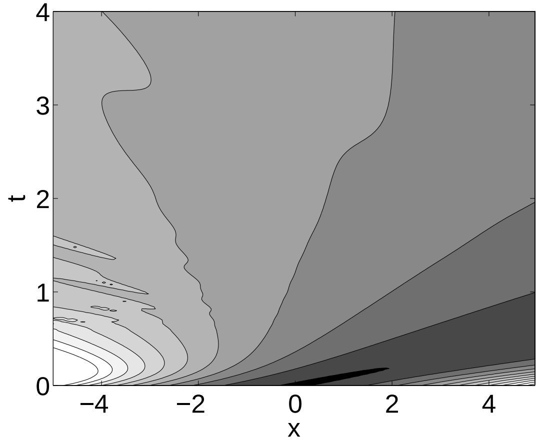
(e) Arnold–Ehrhardt



(f) Di Menza



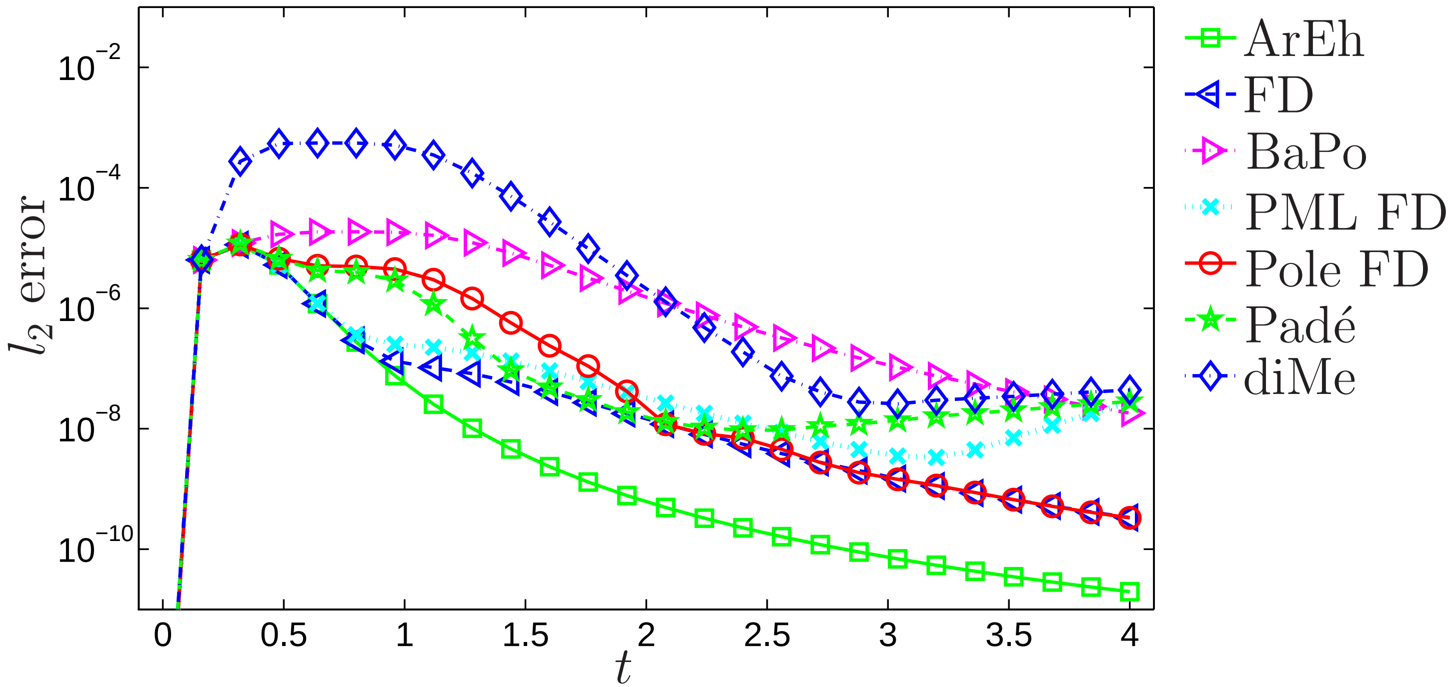
(g) Padé



(h) Szeftel

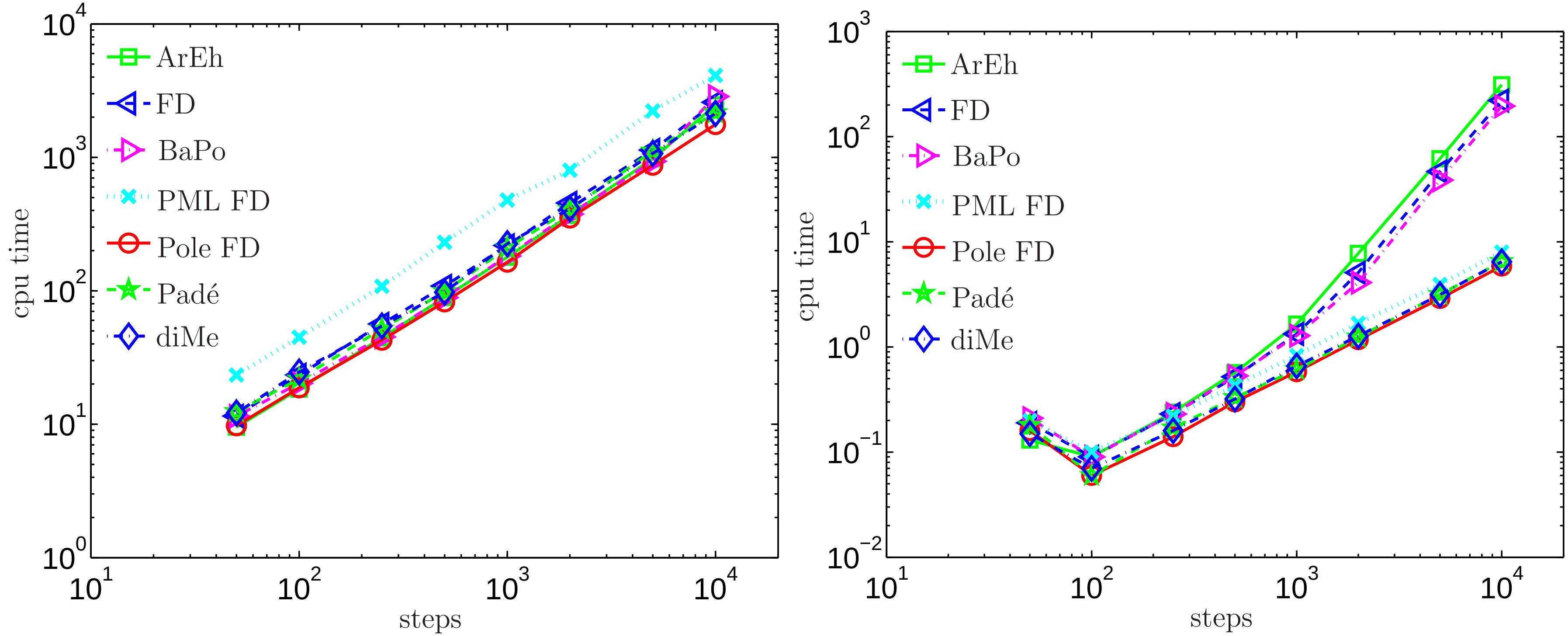
- solutions built with a square root approximation are far better

Example: first group of methods



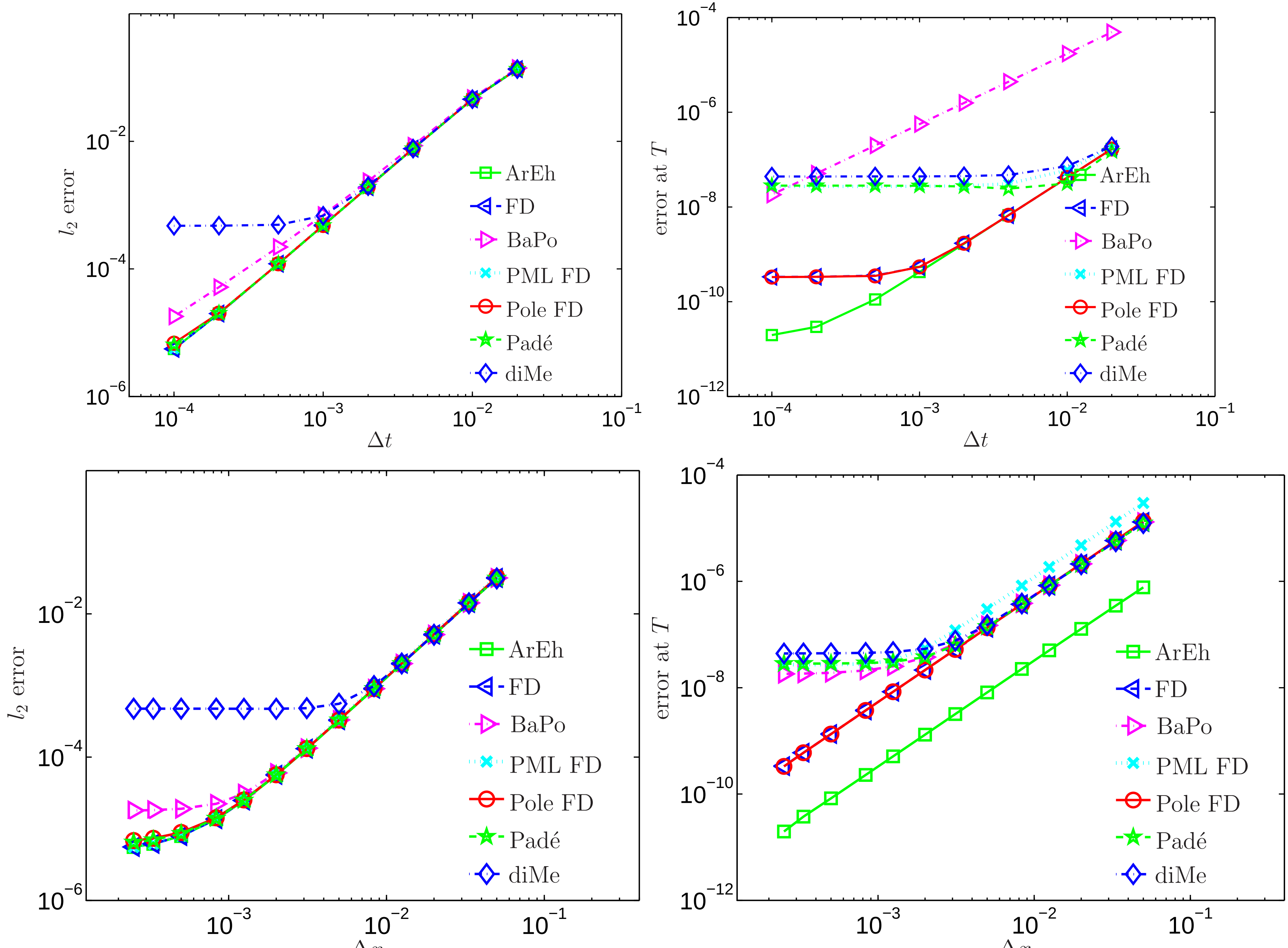
- Time evolution of the spatial l_2 error for various finite difference methods and the fixed step sizes $\Delta x = 2.5 \cdot 10^{-4}$, $\Delta t = 10^{-4}$
- method by Di Menza (**diMe**) shows strong reflection producing an error about 10^2 times larger than the interior discretization error
- method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

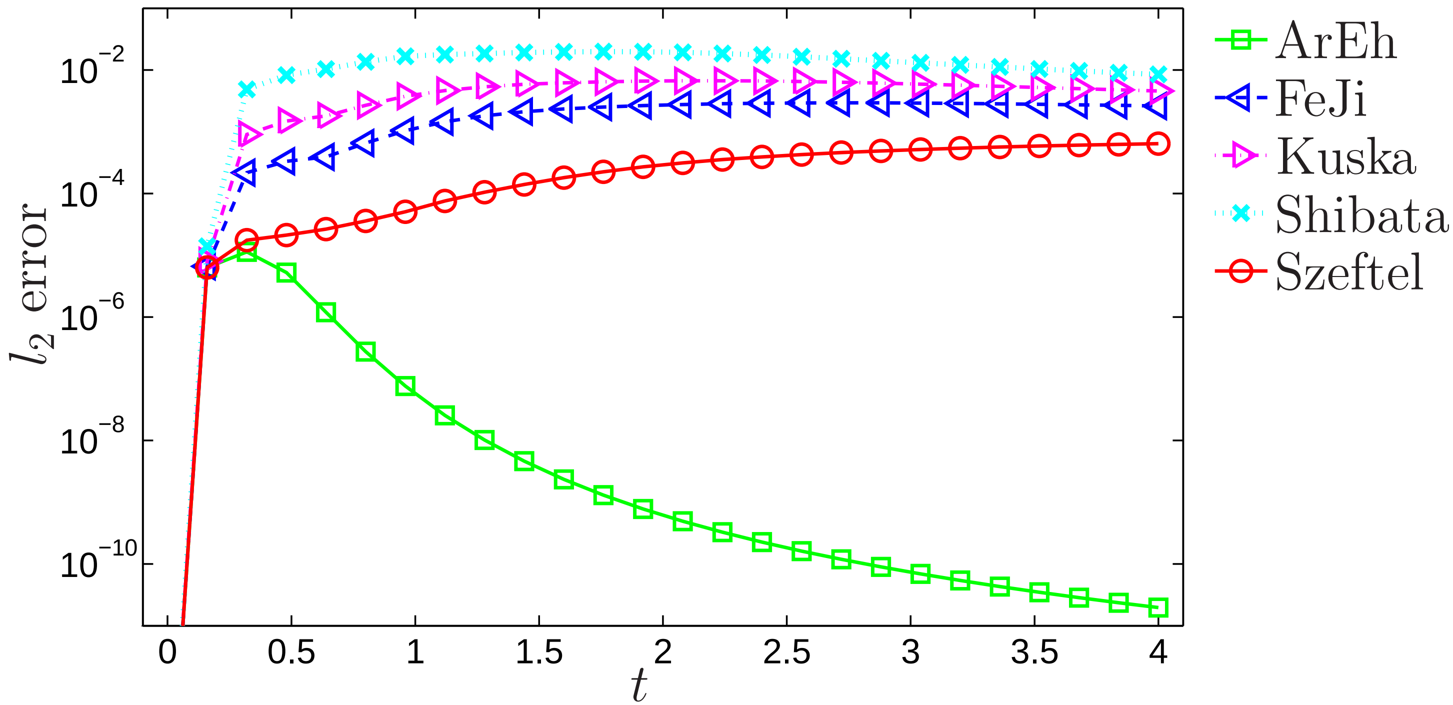


- **left figure:** fine spatial mesh (#unknowns 40.000)
  - solution of the linear system is most time consuming part
    $\Longrightarrow$ the different methods can hardly be distinguished
- **right figure:** coarse spatial mesh (about 200 unknowns)
  - **ArEh**, **FD** and **BaPo** methods do not scale 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!)

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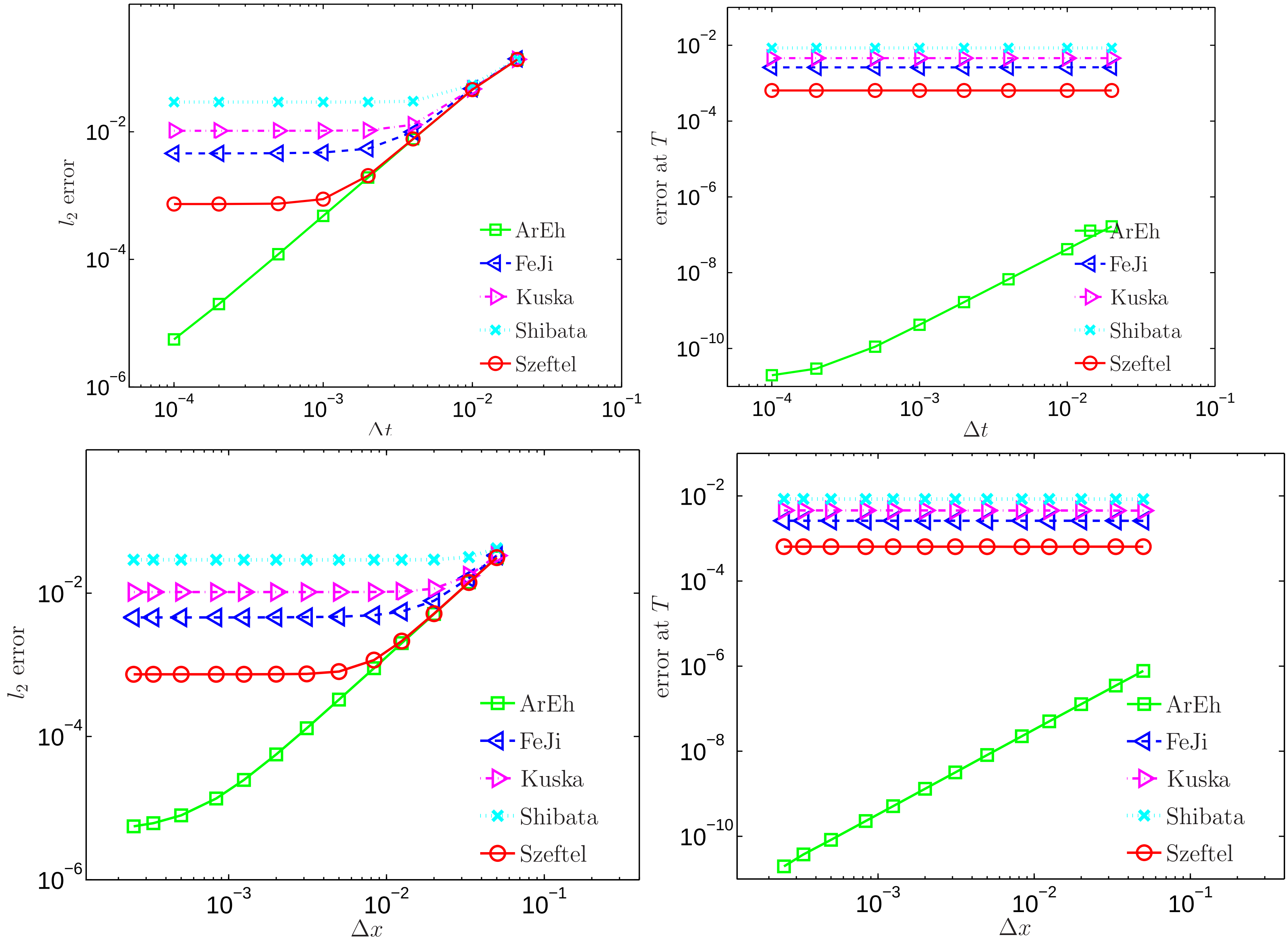
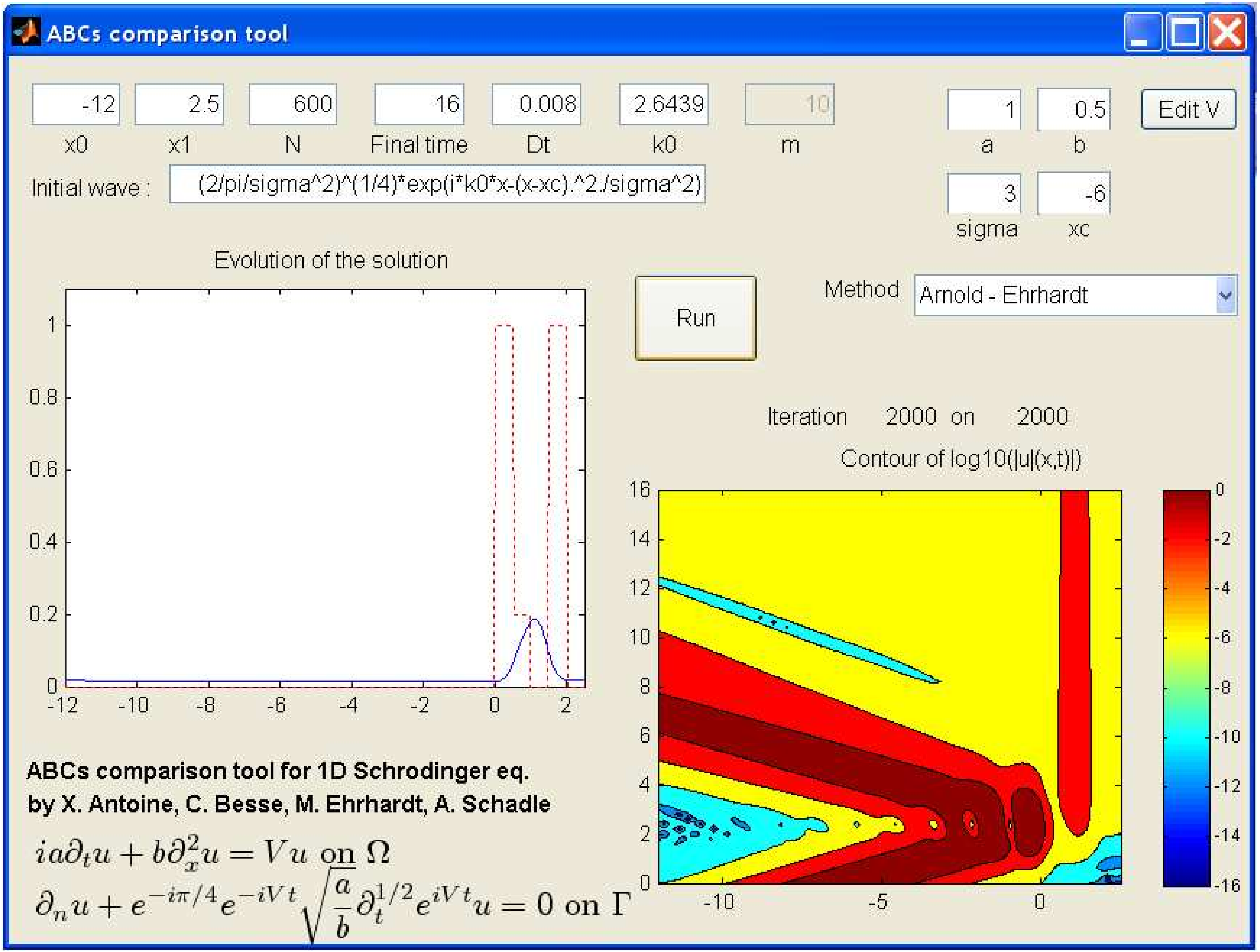


Comparison tool for 1D Schrödinger equation



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!

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- 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
  - paralinearization

  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

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

- Nonlinearity = potential multiplied by the unknown function u
  $\rightsquigarrow$ linear Schrödinger equation with a potential $V(x,t) = \lambda |u(x,t)|^2$

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

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

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

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

The Phase Function Transformation Strategy

We consider the cubic nonlinear Schrödinger equation

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- new unknown function $v(x,t) = e^{i\mathcal{V}(x,t)} u(x,t)$ satisfies

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$\leadsto$ linear variable coefficients Schrödinger equation

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$\rightsquigarrow$ linear variable coefficients Schrödinger equation

- Method of [Engquist & Majda '79] $\rightsquigarrow$ second order absorbing BC

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

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 (cf. review paper for the 2D case)

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Thank You for Your Attention!