convolution quadrature for the linear Schrödinger equation

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joint work with

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Overview

the semidiscrete problem

Schrödinger equation

$$\mathbf{i}\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t) + \mathcal{V}(x)u(x,t) =: \mathbf{H}u, \qquad x \in \mathbb{R}^d,\ t > 0$$

$$u(\cdot, t=0) = u_0.$$

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Theorem (semidiscrete approximation)

Let the potential $\mathcal{V}$ be bounded, and let u_0 be sufficiently smooth. Let the semidiscrete approximations $u^n \approx u(nk)$ be obtained with an A-stable RK or multistep method of order q. Then:

$$\|u^n - u(nk)\|_{L^2(\mathbb{R}^d)} \lesssim Tk^q \|\mathbf{H}^{q+1}u_0\|_{L^2(\mathbb{R}^d)},$$

$$\|u^n - u(nk)\|_{H^1(\mathbb{R}^d)} \lesssim Tk^q \left(\|\mathbf{H}^{q+2}u_0\|_{L^2(\mathbb{R}^d)} + \|\mathbf{H}^{q+1}u_0\|_{L^2(\mathbb{R}^d)}\right).$$

Proof: follows from rational approximations of semigroups.

Problem formulation

- Schrödinger equation

$$\begin{cases} \mathbf{i}\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t) + \mathcal{V}(x)u(x,t)\ , \quad x \in \mathbb{R}^d,\ t \in (0,\infty) \\ u(\cdot, t=0) = u_0. \end{cases}$$

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  - potential $\mathcal{V} \equiv \mathcal{V}_{ext} \in \mathbb{R}$ outside Ω
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- questions:
  - what (transparent) boundary conditions to pose for u^n on $\partial\Omega$? $\rightarrow$ has the form of a DtN operator
  - how to realize the DtN operator? $\rightarrow$ FEM-BEM coupling
  - error and stability analysis?

Multistep methods

$$\mathbf{i}\frac{\partial}{\partial t}u(x,t) = -\Delta u(x,t) + \mathcal{V}(x)u(x,t)$$

- K-step method is given by coefficients
  $\alpha_j, \beta_j \in \mathbb{R}, \quad j = 0, \ldots, K$
- sequence of approximations defined as the solutions of

$$\frac{\mathbf{i}}{k}\sum_{j=0}^{K}\alpha_j u^{n-j} = \sum_{j=0}^{K}\beta_j\left(-\Delta + \mathcal{V}\right)u^{n-j} \qquad \forall n \geq K.$$

Derivation of the boundary conditions

- idea: use the Z-transform: $\hat{u}(z) := \sum_{n=0}^{\infty} u^n z^n$:
- set $\mathbf{H} := -\Delta + \mathcal{V}$

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$\rightarrow$ differential equation for $\hat{u}$:

$$\left(\frac{\mathbf{i}\delta(z)}{k} + \Delta - \mathcal{V} \right) \hat{u}(z) = 0, \qquad \delta(z) := \frac{\sum_{j=0}^{K} \alpha_j z^j}{\sum_{j=0}^{K} \beta_j z^j}$$

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- solution $\hat{u}$ on (x_r, ∞) has form

$$\hat{u}(z;x) = A^+(z)\, e^{\mathbf{i}\sqrt{\mathbf{i}\frac{\delta(z)}{k} - \mathcal{V}_r}\, x} + A^-(z)\, e^{-\mathbf{i}\sqrt{\mathbf{i}\frac{\delta(z)}{k} - \mathcal{V}_r}\, x}$$

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- explicit form of Dirichlet-to-Neumann operator:

$$\mathrm{DtN}\, \hat{u}(z) = \partial_x \hat{u}(z) = \mathbf{i}\sqrt{\mathbf{i}\frac{\delta(z)}{k} - \mathcal{V}_r}\, \hat{u}(z)$$

(note: DtN cannot be realized exactly in higher dimensions)

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$$\sum_{n=0}^{\infty} \psi_n z^n := \mathbf{i}\sqrt{\mathbf{i}\frac{\delta(z)}{k} - \mathcal{V}_r}$$

- Cauchy-product formula gives:

$$\boxed{\partial_x u^n(x) = \sum_{k=0}^{n} \psi_k u^{n-k}(x)}$$

Transparent boundary conditions – Multistep methods 1D

For all $n \geq K$, find u^n such that

$$\begin{cases} \frac{\mathbf{i}}{k} \sum_{j=0}^{K} \alpha_j u^{n-j} = \sum_{j=0}^{K} \beta_j \left(-\partial_x^2 + \mathcal{V}\right) u^{n-j}, & x \in (x_l, x_r), \\ \partial_x u^n(x) = \sum_{k=0}^{n} \psi_k u^{n-k}(x), & x = x_r, \\ \text{analogous b.c. for } x = x_l \end{cases}$$

with

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- m-stage method given by $A \in \mathbb{R}^{m\times m}$, $b \in \mathbb{R}^m$, $c \in \mathbb{R}^m$
- approximation at time $t_{n+1} := t_n + k$ given by:

$$\boldsymbol{U}_i^n = u_n + k \sum_{j=1}^{m} a_{ij} \left(-\mathbf{i}\mathbf{H}\boldsymbol{U}_j^n\right), \qquad i = 1, \dots, m,$$

$$u_{n+1} = u_n + k \sum_{j=1}^{m} b_j \left(-\mathbf{i}\mathbf{H}\boldsymbol{U}_j^n\right)$$

- we only consider A-stable methods with regular matrix A.

RK-method

$$\left(\mathrm{I} + \mathbf{i}kA\underline{\mathbf{H}}\right)\boldsymbol{U}^n = \mathbb{1}u_n$$
$$u^{n+1} = R(\infty) + \boldsymbol{b}^T A^{-1}\boldsymbol{U}^n$$

RK-method, rewritten

$$\left(-\mathbf{i}A^{-1} + k\underline{\mathbf{H}}\right)\boldsymbol{U}^n = u_n\mathbf{d}, \qquad \mathbf{d} = -\mathbf{i}A^{-1}\mathbb{1}$$

update formula: $u^{n+1} = R(\infty) + \boldsymbol{b}^T A^{-1}\boldsymbol{U}^n$

Transparent boundary conditions – RK methods 1D

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where

$$\delta(z) := \left(A + \mathbb{1}\boldsymbol{b}^T \frac{z}{1-z}\right)^{-1},$$

$$\sum_{n=0}^{\infty} \boldsymbol{\Psi}_n^{(l,r)} z^n := \mathbf{i}\sqrt{\frac{\mathbf{i}\delta(z)}{k} - \mathcal{V}_{(l,r)}\boldsymbol{I}}, \qquad \forall |z| < 1,$$

- coefficients $\boldsymbol{\Psi}_n^{(l,r)}$ are now matrices in $\mathbb{C}^{m\times m}$.

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- possible to show optimal convergence

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- solution: approximate Cauchy integral by trapezoidal rule:

$$\mathbf{\Psi}_j = \frac{1}{2\pi\mathbf{i}} \oint_{\lambda\mathbb{T}} f(\zeta)\,\zeta^{-j-1}\,d\zeta \approx \frac{\lambda^{-j}}{Q+1} \sum_{l=0}^{Q} f\left(\lambda\zeta_{Q+1}^{-l}\right)\zeta_{Q+1}^{lj}$$

with $\zeta_{Q+1} := e^{\frac{2\pi\mathbf{i}}{Q+1}}$ and $f(z) := \mathbf{i}\sqrt{\frac{\mathbf{i}\delta(z)}{k} - \mathcal{V}\,\mathrm{I}}$

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- for $Q \geq j$: exponential convergence, $\left\|\tilde{\mathbf{\Psi}}_j - \mathbf{\Psi}_j\right\| \leq \frac{C}{\sqrt{k}} \frac{\lambda^{Q+1}}{1-\lambda^{Q+1}}$

Stability under quadrature – 1D

Theorem

Let $\mathcal{V}$ *be bounded,* $nk \leq T$, $\max_{j=1\dots n} \left\| \boldsymbol{\psi}_j - \tilde{\boldsymbol{\psi}}_j \right\| \leq Ck^{3/2}$.
Then there exists a constant $C(T) > 0$ *such that:*

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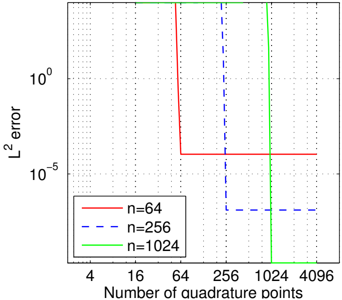
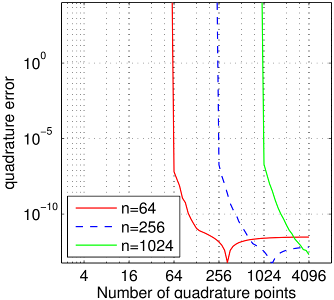
Idea of proof: boundary conditions are not local in time
$\Rightarrow$ rewrite as a full space problem that is local in time and can be analyzed as a time stepping scheme

details

Stability under quadrature of the solution – 1D

- using $Q = n$ quadrature points is nessary
- this condition is also (practically) sufficient





3-stage Radau IIA, $p = 4$, $h = k$;

L^2-error = maximal L^2-error over all time steps; quadrature error = maximal error over all weights

higher spatial dimensions

- Z transform $\hat{\boldsymbol{U}}$ of stages solves Helmholtz equation

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- FEM-BEM coupling problem in each step (here: symmetric coupling)

details

multi-d formulation with symmetric coupling

$$(\mathrm{I} + \mathbf{i}kA\underline{\mathbf{H}})\,\boldsymbol{U}^n = u^n \mathbb{1} \qquad \text{in } \Omega,$$

$$\partial_n^+ U^n = \sum_{j=0}^{n} (-1/2 + K_j^T)\phi^{n-j} - W_j \gamma^- U^{n-j}$$

$$\sum_{j=0}^{n} V_j \phi^{n-j} = \sum_{j=0}^{n} (-1/2 + K_j)\gamma^- U^{n-j}$$

$$u^{n+1} = R(\infty)u^n + b^T A^{-1}\boldsymbol{U}^n$$

discretization:

- FEM based on $X_h \subset H^1(\Omega)$ for stage vector $\boldsymbol{U}^n$
- FEM-BEM coupling based on $Y_h \subset H^{-1/2}(\partial\Omega)$ for ϕ^n

Theorem

Let u^n, $\boldsymbol{U^n} \in H^1(\mathbb{R}^d)$ *be the semidiscrete approximations and stage vectors. Let potential* $\mathcal{V} \in L^\infty(\mathbb{R}^d)$. *Assume*

$$\inf_{w_h \in X_h} \|u - w_h\|_{L^2(\Omega)} \le C k^{1/2} \|u\|_{H^1(\Omega)} \qquad \forall u \in H^1(\Omega).$$

Then:

$$\|u^n - u_h^n\|_{H^1(\Omega)} \lesssim$$

$$k \sum_{j=0}^{n-1} \inf_{x_h \in X_h} \|\underline{\mathbf{H}}\boldsymbol{U}^j - x_h\|_{H^1(\Omega)} + k \sum_{j=0}^{n-1} \inf_{x_h \in X_h} \|\boldsymbol{U}^j - x_h\|_{H^1(\Omega)} +$$

$$k \sum_{j=0}^{n-1} \inf_{y_h \in Y_h} \|\partial_n^+ \underline{\mathbf{H}}\boldsymbol{U}^j - y_h\|_{H^{-1/2}(\Gamma)} + k \sum_{j=0}^{n-1} \inf_{y_h \in Y_h} \|\partial_n^+ \boldsymbol{U}^j - y_h\|_{H^{-1/2}(\Gamma)}$$

Corollary

- q = *order of the RK-method*
- *FEM space = p.w. polynomials of degree* p_1 *on mesh, size* h_1
- *BEM space = p.w. polynomials of degree* p_0 *on mesh, size* h_0
- u_0 *sufficiently smooth*

Then:

$$\|u(nk) - u_h^n\|_{H^1(\Omega)} \leq CT\left[k^q + h_1^{p_1} + h_0^{p_0+3/2}\right].$$

analysis of the method

- analysis is performed in a time stepping manner

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  $(-\mathbf{i}A^{-1}\boldsymbol{U},\boldsymbol{V})_{L^2(\Omega)} + k(\nabla\boldsymbol{V},\nabla\boldsymbol{V})_{L^2(\Omega)} + k(\mathcal{V}\boldsymbol{U},\boldsymbol{V})_{L^2(\Omega)}$

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- method (both discrete and continuous):

$$a_{\Omega,\mathcal{V}}(\boldsymbol{U}^n,\boldsymbol{V}) + \text{convolution terms} = (u^n\mathbf{d},\boldsymbol{V})_{L^2(\Omega)} \qquad \forall\boldsymbol{V}$$

$$u^{n+1} = R(\infty)u^n + \boldsymbol{b}^T A^{-1}\boldsymbol{U}^n$$

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- rephrase the convolution parts by auxiliary local-in-time terms:

$$a_{\Omega,\mathcal{V}}(\boldsymbol{U}^n,\boldsymbol{V}) + a_{\mathbb{R}^d\setminus\Gamma,\mathcal{V}_{ext}}(\boldsymbol{U}^n_*,\boldsymbol{V}_*) = (u^n\mathbf{d},\boldsymbol{V})_{L^2} + (u^n_*\mathbf{d},\boldsymbol{V}_*)_{L^2}$$
$$u^{n+1} = R(\infty)u^n + \boldsymbol{b}^T A^{-1}\boldsymbol{U}^n$$
$$u^{n+1}_* = R(\infty)u^n_* + \boldsymbol{b}^T A^{-1}\boldsymbol{U}^n_*$$

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$$u^{n+1} = R(\infty)u^n + \boldsymbol{b}^T A^{-1}\boldsymbol{U}^n, \qquad u_*^{n+1} = R(\infty)u_*^n + \boldsymbol{b}^T A^{-1}\boldsymbol{U}_*^n$$

$$B((\boldsymbol{U},\boldsymbol{U}_*),(\boldsymbol{V},\boldsymbol{V}_*)) := a_{\Omega,\mathcal{V}}(\boldsymbol{U},\boldsymbol{V}) + a_{\mathbb{R}^d\setminus\Gamma,\mathcal{V}_{ext}}(\boldsymbol{U}_*,\boldsymbol{V}_*)$$

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correct ansatz and test spaces

Let $X_h \subseteq H^1(\Omega)$, $Y_h \subseteq H^{-1/2}(\Gamma)$. Set

$$\widehat{H}(X_h,Y_h) := \{(v,v_*) \in X_h \times H^1(\mathbb{R}^d\setminus\Gamma) \quad : \quad [\![\gamma v_*]\!] = -\gamma^- v \quad \text{and} \quad \gamma^- v_* \in Y_h^\circ\}.$$

analysis of the method

$$a_{\Omega,\mathcal{V}}(\boldsymbol{U}^n, \boldsymbol{V}) + a_{\mathbb{R}^d\setminus\Gamma,\mathcal{V}_{ext}}(\boldsymbol{U}^n_*, \boldsymbol{V}_*) = (u^n \mathbf{d}, \boldsymbol{V})_{L^2} + (u^n_* \mathbf{d}, \boldsymbol{V}_*)_{L^2} \qquad \forall \boldsymbol{V}$$

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notation for $(\boldsymbol{U},\boldsymbol{U}_*) \in \underline{H^1(\Omega)} \times \underline{H^1(\mathbb{R}^d\setminus\Gamma)}$:

- $\|(\boldsymbol{U},\boldsymbol{U}_*)\|_{L^2} := \|\boldsymbol{U}\|_{L^2(\Omega)} + \|\boldsymbol{U}_*\|_{L^2(\mathbb{R}^d)}$
- $\|(\boldsymbol{U},\boldsymbol{U}_*)\|_{H^1} := \|\boldsymbol{U}\|_{H^1(\Omega)} + \|\boldsymbol{U}_*\|_{H^1(\mathbb{R}^d\setminus\Gamma)}$

Convergence of fully discrete scheme

$$B((\boldsymbol{U},\boldsymbol{U}_*),(\boldsymbol{V},\boldsymbol{V}_*)) := a_{\Omega,\mathcal{V}}(\boldsymbol{U},\boldsymbol{V}) + a_{\mathbb{R}^d\setminus\Gamma,\mathcal{V}_{ext}}(\boldsymbol{U}_*,\boldsymbol{V}_*)$$

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Theorem (local-in-time representation)

The recursion: Find $(\boldsymbol{U}_h^n,\boldsymbol{U}_*^n) \in \underline{\widehat{H}(X_h,Y_h)}$ *s.t.*

$$\begin{cases} B((\boldsymbol{U}_h^n,\boldsymbol{U}_*^n),(\boldsymbol{V},\boldsymbol{V}_*)) = l(\boldsymbol{V},\boldsymbol{V}_*) \qquad \forall(\boldsymbol{V},\boldsymbol{V}_*) \in \underline{\widehat{H}(X_h,Y_h)} \\ + \text{ update formulas for } u^n,\ u_*^n \end{cases}$$

reproduces the stage vectors $\boldsymbol{U}_h^n$ *of the RKCQ. Furthermore,* $[\![\partial_n \boldsymbol{U}_*^n]\!] = -\phi_h^n$.

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$\rightsquigarrow$ stability analysis for B?

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The recursion: Find $(\boldsymbol{U}^n_h,\boldsymbol{U}^n_*) \in \underline{\widehat{H}(X_h,Y_h)}$ *s.t.*

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$\rightsquigarrow$ stability analysis for B?

note: $\widehat{H}(X_h,Y_h) \not\subset \widehat{H}(H^1(\Omega),H^{-1/2}(\Gamma))$
$\rightsquigarrow$ analysis will require additional consistency errors

Theorem (stability)

Consider the sequence

$$\begin{cases} B((\boldsymbol{U}_h^n, \boldsymbol{U}_*^n), \cdot) = l(\cdot) + (\mathbf{F}_n, \cdot), \\ +\textit{update formulas for } u^n,\, u_*^n \end{cases} \qquad n = 0, 1, \ldots,$$

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(i) *Let* $\mathbf{F}_n \in L^2 \quad \forall n$. *Then* $\|u_h^n\|_{L^2} \leq \|u_h^0\|_{L^2} + C \sum_{j=0}^{n-1} \|\mathbf{F}_n\|_{L^2}$

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(ii) $\mathbf{F}_n \in H^1 \quad \forall n$. *Then*

$$\|u_h^n\|_{H^1} \leq \|u_h^0\|_{H^1} + C \sum_{j=0}^{n-1} \inf_{\mathbf{w}_h} \left[\|\mathbf{w}_h\|_{H^1} + k^{-1/2} \|\mathbf{F}_n - \mathbf{w}_h\|_{H^1} \right]$$

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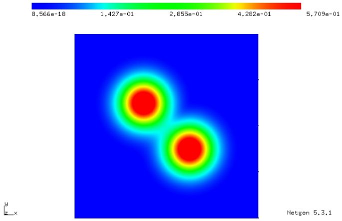
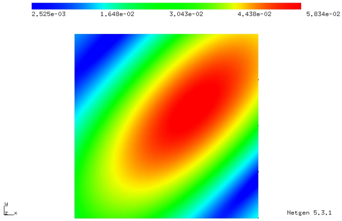
Key ingredient of the proof:

- express B^{-1} in terms of a self-adjoint operator $\mathcal{T}$
- with spectral theorem express B^{-1} as a multipl. oper. with a fct. g
- g can be expressed through R. Use $|R(z)| \leq 1$ on imaginary axis

solution at $t = 0$ (left) and $t = 2$ (right)





solution is sum of two Gaussian beams: $u_{ex} = u_{ex}^1 + u_{ex}^2$

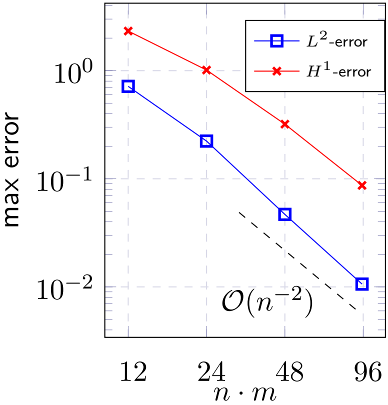
with

$$u_{ex}^i(x,t) = \sqrt[4]{\frac{2}{\pi}}\sqrt{\frac{\mathbf{i}}{-4t+\mathbf{i}}}\exp\left(\frac{-\mathbf{i}\left|x - x_c^i\right|^2 - \mathbf{p}_0^i\cdot(x - x_c^i) + \left|\mathbf{p}_0^i\right|^2 t}{-4t+\mathbf{i}}\right),$$

$$x_c^1 = (-1,1,0), \qquad \mathbf{p}_0^1 = (1,0,0)$$
$$x_c^2 = (1,-1,0), \qquad \mathbf{p}_0^2 = (0,0,0)$$

modulus of solution on slize $z = 0$ is shown

"symmetric coupling"

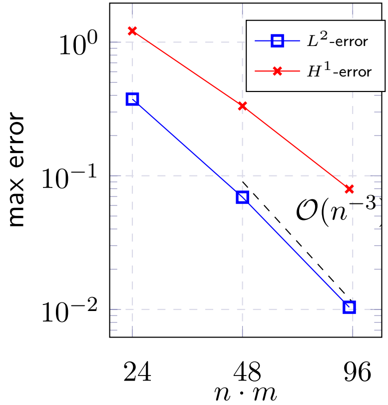


implementation details:

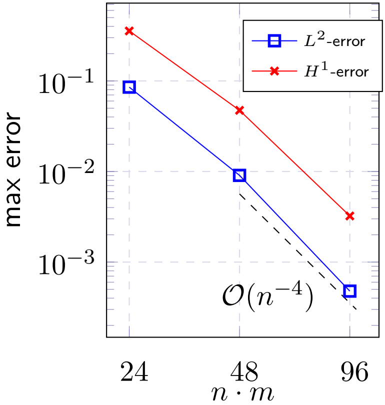
- n = number steps
- m = number stages
- $\Omega = (-4,4)^3$
- $T = 2$
- $h = k$
- p_{FEM} = time order
- $p_{BEM} = p_{FEM} - 1$
- $\rightarrow$ space discret. matches temporal order
- FEM = Netgen/NgSolve
- BEM = BEM++
- problem size (per stage) for 2-stage Radau IIA: X_h has 900k DOF, Y_h has 73k DOF, 200k tets, 12k bdy triangles

1 stage Gauss (order 2)

"symmetric coupling", cont'd



2 stage Radau IIA (order 3)



3 stage Radau IIA (order 5)

"Johnson-Nédélec coupling"

time steps	DOF (FEM)	max L^2 error	rate	max H^1 error	rate
8	2.197	0.182747	—	0.917963	—
16	15.625	0.297628_{-1}	6.1	0.276579	3.3
32	117.649	0.193383_{-2}	15.4	0.436807_{-1}	6.3
64	912.673	0.118364_{-3}	16.3	0.567161_{-2}	7.7

geometry: cube (side length 6);
2-stage Radau IIA, $h = k$
FEM with $p = 3$
BEM with $p = 2$; Johnson-Nédélec coupling
smooth solution; end time: $T = 1$

computations: NETGEN/NGSOLVE and BEM++

Summary and outlook

Summary:

- infinite domain $\rightarrow$ introduce artificial boundary
- Z-transform yields transparent b.c. via Helmholtz problems
- Runge Kutta methods for high order
- discrete stability $\rightarrow$ method stable under quadrature errors
- full order in space and time

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- infinite domain $\rightarrow$ introduce artificial boundary
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- full order in space and time

outlook:

- compression techniques
- extension of discrete stability analysis for high order RK convolution quadrature to wave equation

higher spatial dimensions: b.c. for the stage vector $\boldsymbol{U}^n$

- $\delta(z) = \left(A + \frac{z}{1-z} \mathbb{1} b^\top \right)^{-1}$
- Z-transform of stage vectors $\hat{\boldsymbol{U}}$ solves Helmholtz equation

$$-\Delta\hat{\boldsymbol{U}} + \underbrace{\left(-\frac{\mathbf{i}\delta(z)}{k} + \mathcal{V}_{ext} \right)}_{=:B^2(z)} \hat{\boldsymbol{U}} = 0 \quad \text{in } \mathbb{R}^d \setminus \overline{\Omega} \qquad (1)$$

- fact: $\sigma(B(z)) \subset \mathbb{C}^+$

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- fact: $\sigma(B(z)) \subset \mathbb{C}^+$
- the DtN^+ map for (1) can be expressed by "classical" integral operators K, K^T, V, and W (all depending on $B(z)$)

$$-\mathrm{DtN}^+ := W + \left(-\frac{1}{2} + K^T\right)V^{-1}\left(-\frac{1}{2} + K\right),$$

transparent b.c. in higher dimensions, cont'd

$$-\mathrm{DtN}^{+} := W + \left(-\frac{1}{2} + K^{T}\right) V^{-1} \left(-\frac{1}{2} + K\right),$$

- symmetric coupling introduces additional variable $\hat{\phi} := V^{-1}(-1/2 + K)\hat{U}$ to lead to the system:

$$-\mathrm{DtN}\,\hat{\boldsymbol{U}} = W\hat{\boldsymbol{U}} + \left(-\frac{1}{2} + K^{T}\right)\hat{\phi}, \qquad V\hat{\phi} = \left(-\frac{1}{2} + K\right)\hat{\boldsymbol{U}}$$

- inverse Z-transformation yields (with computable) operators K_j, K_j^T, W_j, V_j:

$$\partial_n^{+}\boldsymbol{U}^{n} = \sum_{j=0}^{n}(-1/2 + K_j^{T})\phi^{n-j} - W_j\gamma^{-}\boldsymbol{U}^{n-j}$$

$$\sum_{j=0}^{n} V_j\phi^{n-j} = \sum_{j=0}^{n}(-1/2 + K_j)\gamma^{-}\boldsymbol{U}^{n-j}$$

back

Theorem (convergence in h and k in 1D)

Let potential $\mathcal{V} \in W^{1,\infty}(\mathbb{R}^1)$.
Let $X_h \subset H^1(\Omega)$ *and let the A-stable RK method have order* q.
Let u_0 *be sufficiently smooth. Then:*

$$\|u_h^n - u(nk)\|_{H^1(\Omega)} \preceq k \sum_{j=0}^{n-1} \inf_{x_h \in X_h} \left\| \boldsymbol{U}^j - x_h \right\|_{H^1(\Omega)} + k \sum_{j=0}^{n-1} \inf_{x_h \in X_h} \left\| \underline{\mathbf{H}} \boldsymbol{U}^j - x_h \right\|_{H^1(\Omega)} + k^q \left(\|\mathbf{H}^{q+2} u_0\|_{L^2(\mathbb{R})} + \|\mathbf{H}^{q+1} u_0\|_{L^2(\mathbb{R})} \right)$$

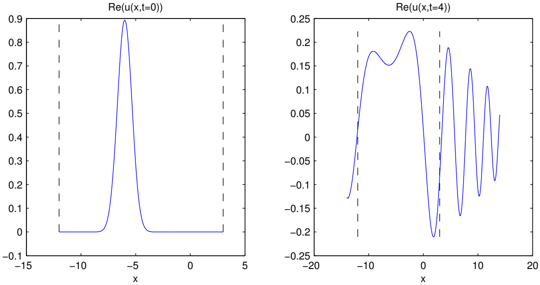
corollary

$X_h =$ space of piecewise polynomials of degree p. Then:

$$\sup_{n:nk<T} \|u_h^n - u(nk)\|_{H^1(\Omega)} \leq C \left[k^q + h^p \right].$$

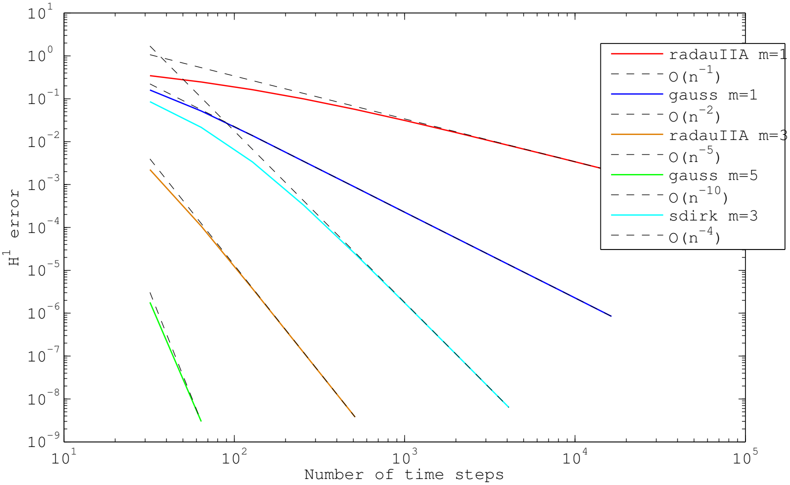
Numerical example – 1D

- consider the initial condition u_0 as a Gaussian distribution
- $\mathcal{V} \equiv 0$
- exact solution is known

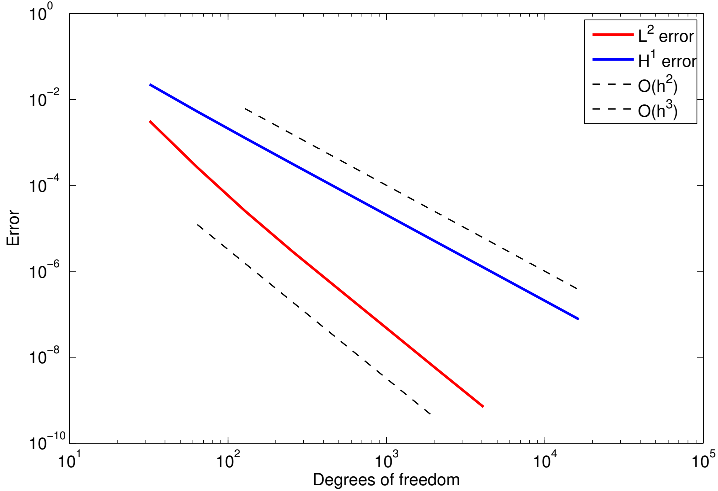


- compare behavior of different numerical schemes

Numerical example – 1D



Spatial convergence



$p = 2$ in space, 5-stage Gauss in time, $h = k$

back

Stability 1D – Proof

- consider solutions to

$$\left(\boldsymbol{I} + \mathbf{i}kA\underline{\mathbf{H}}_h\right)\boldsymbol{E}^n(x) = e_n(x)\mathbb{1} + \tau_n, \quad x \in (x_l, x_r),$$

$$\partial_n \boldsymbol{E}^n(x) = \sum_{j=0}^{n} \boldsymbol{\Psi}_k \boldsymbol{E}^{n-j}.$$

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$$\partial_n \boldsymbol{E}^n(x) = \sum_{j=0}^{n} \boldsymbol{\Psi}_k \boldsymbol{E}^{n-j}.$$

- extend the solution to the whole space:

$$\begin{aligned}(\boldsymbol{I} + \mathbf{i}kA\underline{\mathbf{H}})\boldsymbol{W}^n(x) &= w_n(x)\mathbb{1}, && x \in \mathbb{R} \setminus [x_l, x_r],\\ \boldsymbol{W}^n &= E_n && x \in \{x_l, x_r\}\end{aligned}$$

Stability 1D – Proof

- consider solutions to

$$(\boldsymbol{I} + \mathbf{i}kA\underline{\mathbf{H}}_h)\,\boldsymbol{E}^n(x) = e_n(x)\mathbb{1} + \tau_n, \quad x \in (x_l, x_r),$$

$$\partial_n \boldsymbol{E}^n(x) = \sum_{j=0}^{n} \boldsymbol{\Psi}_k \boldsymbol{E}^{n-j}.$$

- extend the solution to the whole space:

$$\begin{aligned}(\boldsymbol{I} + \mathbf{i}kA\underline{\mathbf{H}})\boldsymbol{W}^n(x) &= w_n(x)\mathbb{1}, & x &\in \mathbb{R} \setminus [x_l, x_r],\\ \boldsymbol{W}^n &= E_n & x &\in \{x_l, x_r\}\end{aligned}$$

$$\Rightarrow \partial_n \boldsymbol{W}^n = \sum_{n=0}^{\infty} \boldsymbol{\Psi}_k \boldsymbol{W}^{n-j} = \sum_{n=0}^{\infty} \boldsymbol{\Psi}_k \boldsymbol{W}^{n-j}$$

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- combining gives:

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- structurally like one RK-step for whole-space Schrödinger equation

back

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- use stability function of method $R(z)$.

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- $\|e_{n+1}\| \leq \|e_n\| + \|\tau_n\|$

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