A space–time Trefftz discontinuous Galerkin method for the linear Schrödinger equation

Sergio Gómez[1,*], Andrea Moiola[1]
[1]Dipartimento di Matematica "F. Casorati", Università di Pavia, 27100 Pavia, Italy
*Email: sergio.gomez01@universitadipavia.it

Abstract

A space–time Trefftz discontinuous Galerkin method for the Schrödinger equation with piecewise-constant potential is presented. Trial and test spaces are spanned by non-polynomial complex wave functions that satisfy the Schrödinger equation locally on each element of the space–time mesh. We prove well-posedness and stability of the method, and optimal, high-order, h-convergence error estimates in a skeleton norm. We validate numerically our theoretical results presented.
Keywords: Linear Schrödinger equation, Trefftz method, discontinuous Galerkin method.

1 Introduction

In this work we consider the following initial boundary value problem for the homogeneous, time-dependent Schrödinger equation on a space–time cylinder $Q = \Omega \times I$, where Ω is an open and bounded domain in $\mathbb{R}^d$, $d \in \mathbb{N}$, with Lipschitz boundary $\partial\Omega$ and $I = (0, T)$, for some $T > 0$:

$$
\begin{aligned}
i\partial_t \psi + \Delta\psi - V\psi &= 0, && \text{in } Q, && (1.1a)\\
\psi &= g_{\mathrm{D}} && \text{on } \partial\Omega \times I, && (1.1b)\\
\psi(\mathbf{x}, 0) &= \psi_0(\mathbf{x}), && \text{on } \Omega. && (1.1c)
\end{aligned}
$$

Here the Dirichlet boundary datum g_{D} and the initial condition ψ_0 are given functions; $V : \Omega \to \mathbb{R}$ is a piecewise-constant potential and the Laplacian operator Δ refers to the space variable $\mathbf{x}$ only.

The model (1.1) arises from a wide number of applications: it is the fundamental equation of quantum mechanics, in optics it is known as "paraxial wave equation" and approximates the Helmholtz equation when the optical field acts mostly along one specific axis (Fresnel's approximation), while in underwater acoustics it is called "parabolic equation".

We present the main details in the formulation and the analysis of the space–time Trefftz-DG method for the linear Schrödinger equation proposed in [2].

2 Trefftz-DG formulation

Let $\mathcal{T}_h(Q)$ be a space–time finite element mesh of Q, where each element $K \in \mathcal{T}_h(Q)$ has a tensor product structure $K = K_{\mathbf{x}} \times I_n$ with $K_{\mathbf{x}}$ being an element of a polytopic partition of Ω and I_n is an interval in time.

The global Trefftz space $\mathbf{T}(\mathcal{T}_h)$ consists of functions whose restriction to each cell $K \in \mathcal{T}_h(Q)$ belongs to the following space

$$
\mathbf{T}(K) := \Big\{ w \in H^1\left(I_n; L^2(K_{\mathbf{x}})\right) \cap L^2\left(I_n; H^2\left(K_{\mathbf{x}}\right)\right) \\ \text{s.t. } i\partial_t w + \Delta w - V w = 0 \ \text{ on } K = K_{\mathbf{x}} \times I_n \Big\}.
$$

We consider a finite-dimensional subspace $\mathbb{T}_p\left(\mathcal{T}_h\right) := \prod_{K\in\mathcal{T}_h} \mathbb{T}_p(K) \subset \mathbf{T}(\mathcal{T}_h)$ defined for each $K = K_{\mathbf{x}} \times I_n \in \mathcal{T}_h(Q)$ and for $p \in \mathbb{N}$ as the following set of complex exponentials:

$$
\begin{aligned}
\mathbb{T}_p(K) &:= \operatorname{span}\left\{\phi_\ell(\mathbf{x}, t),\ \ell = 1, \dots, n_{d,p}\right\}, \text{ where}\\
\phi_\ell(\mathbf{x}, t) &:= \exp\left[i \left(k_\ell \mathbf{d}_\ell^\top \mathbf{x} - (k_\ell^2 + V|_K) t \right) \right]\\
&\quad \text{for } \ell = 1, \dots, n_{d,p},
\end{aligned}
$$

for some parameters $\{k_\ell\} \subset \mathbb{R}$ and directions $\{\mathbf{d}_\ell\} \subset \mathcal{S}_1^d := \{\mathbf{v} \in \mathbb{R}^d, |\mathbf{d}| = 1\}$, which can be chosen differently in each cell K. Since each ϕ_ℓ solves (1.1a) in K, it is clear that $\mathbb{T}_p(K)$ is a Trefftz space.

As numerical fluxes we use an upwind in time and classical average in space with an appropriate complex penalization. The Trefftz-DG variational formulation is: seek $\psi_{hp} \in \mathbb{T}_p(\mathcal{T}_h)$ such that $\mathcal{A}\left(\psi_{hp}; s_{hp}\right) = \ell(s_{hp}),\ \forall s_{hp} \in \mathbb{T}_p(\mathcal{T}_h)$, where

$$
\begin{aligned}
\mathcal{A}\left(\psi_{hp}; s_{hp}\right) &:= \int_{\mathcal{F}_h^{\mathrm{D}}} \left(\nabla\psi_{hp} \cdot \vec{\mathbf{n}}_\Omega^x + i\alpha\psi_{hp}\right) \overline{s_{hp}}\, \mathrm{d}S\\
&+ \int_{\mathcal{F}_h^{\mathrm{time}}} \Big(\{\!\{\nabla\psi_{hp}\}\!\} \cdot [\![\overline{s_{hp}}]\!]_{\mathbf{N}} + i\alpha\, [\![\psi_{hp}]\!]_{\mathbf{N}} \cdot [\![\overline{s_{hp}}]\!]_{\mathbf{N}}\\
&- \{\!\{\psi_{hp}\}\!\}\, [\![\nabla\overline{s_{hp}}]\!]_{\mathbf{N}} + i\beta\, [\![\nabla\psi_{hp}]\!]_{\mathbf{N}}\, [\![\nabla\overline{s_{hp}}]\!]_{\mathbf{N}} \Big)\, \mathrm{d}S\\
&\int_{\mathcal{F}_h^{\mathrm{space}}} i\psi_{hp}^-\, [\![\overline{s_{hp}}]\!]_t\, \mathrm{d}\mathbf{x} + \int_{\mathcal{F}_h^T} i\psi_{hp}\overline{s_{hp}}\, \mathrm{d}\mathbf{x},\\
\ell(s_{hp}) &:= \int_{\mathcal{F}_h^0} i\psi_0\overline{s_{hp}}\, \mathrm{d}\mathbf{x}\\
&+ \int_{\mathcal{F}_h^{\mathrm{D}}} g_{\mathrm{D}} \left(\nabla\overline{s_{hp}} \cdot \vec{\mathbf{n}}_\Omega^x + i\alpha\overline{s_{hp}}\right) \mathrm{d}S.
\end{aligned}
$$

As a result of the Trefftz property, the definitions of $\mathcal{A}(\cdot;\cdot)$ and $\ell(\cdot)$ in the variational formulation are independent of the potential V, which has an effect only on the discrete space.

Well-posedness and a quasi-optimality estimate follow from the Lax–Milgram theorem and the coercivity and continuity of $\mathcal{A}(\cdot;\cdot)$.

3 Approximation estimate

The key idea to establish convergence rates in the mesh size h was introduced by O. Cessenat and B. Després in the proof of [1, Thm.3.7] (in the case of the ultra weak variational formulation applied to the Helmholtz equation): if, given any smooth PDE solution ψ, the local discrete space contains an element with the same degree-p Taylor polynomial of ψ, then the space enjoys the same h-approximation properties of the space $\mathbb{P}^p$ of degree-p polynomials. The following condition implies that for any sufficiently smooth Schrödinger solution ψ such an approximant exists in the local Trefftz space.

Condition 1 *Let $B \subset K$ be a $(d{+}1)$-dimensional ball such that K is star-shaped with respect to B. Let $\{\phi_1, \ldots, \phi_{n_{d,p}}\} \subset \mathcal{C}^\infty(K)$ be a basis of $\mathbb{T}^p(K)$. For every $\psi \in \mathbf{T}(K) \cap H^{p+1}(K)$, there exists a complex vector-valued function $\mathbf{a} \in L^1(B)^{n_{d,p}}$ satisfying the following two conditions*

$$\text{For all } |\boldsymbol{j}| \le p \quad \text{and a.e. } (\mathbf{z}, s) \in B,$$
$$D^{\boldsymbol{j}}\psi(\mathbf{z}, s) = \sum_{\ell=1}^{n_{d,p}} a_\ell(\mathbf{z}, s) D^{\boldsymbol{j}}\phi_\ell(\mathbf{z}, s),$$
$$\| |\mathbf{a}|_1 \|_{L^1(B)} \le C_\star |K|^{1/2} \|\psi\|_{H^{p+1}(K)},$$

where $C_\star > 0$ might depend on d, p, and $\{\phi_\ell\}$ but is independent of K and ψ.

Theorem 1 provides the error estimate for the Trefftz-DG approximation of (1.1) in the mesh skeleton norm $|||\cdot|||_{\mathrm{DG}}$ (defined in [2]) assuming that Condition 1 holds true. A key ingredient in the proof consists of estimating the approximation properties of the discrete Trefftz function

$$\Phi(\mathbf{x}, t) := \frac{1}{|B|} \sum_{\ell=1}^{n_{d,p}} \left(\int_B a_\ell(\mathbf{z}, s)\, \mathrm{d}V(\mathbf{z}, s) \right) \phi_\ell(\mathbf{x}, t).$$

Theorem 1 *Let $p \in \mathbb{N}$. Let $\psi \in \mathbf{T}(\mathcal{T}_h) \cap H^{p+1}(\mathcal{T}_h)$ be the exact solution of (1.1) and $\psi_{hp} \in \mathbb{T}_p(\mathcal{T}_h)$ be the Trefftz-DG solution with $\mathbb{T}_p(\mathcal{T}_h)$ satisfying Condition 1 for all $K \in \mathcal{T}_h(Q)$. Set the stabilization parameters α and β as in [2], then there exists a constant C independent of the mesh size such that*

$$|||\psi - \psi_{hp}|||_{\mathrm{DG}} \le C \sum_{K \in \mathcal{T}_h(Q)} h_K^p \|\psi\|_{H^{p+1}(K)},$$

where $h_K := \max\{h_{K_\mathbf{x}}, h_n\}$.

In [2] we prove that Condition 1 is indeed true for the $(1+1)$ and $(2+1)$ dimensional cases under some restrictions of the tuning parameters k_ℓ and $\mathbf{d}_\ell$ for our basis choice.

4 Numerical experiments

We consider the $(1{+}1)$-dimensional Schrödinger equation (1.1) on $Q = (-2, 2) \times (0, 1)$ with homogeneous Dirichlet boundary conditions and the following square-well potential:

$$V(x) = \begin{cases} 0, & x \in (-1, 1), \\ V_*, & x \in (-2, 2) \setminus (-1, 1), \end{cases}$$

for some $V_* > 0$. The initial condition is taken as an eigenfunction of $-\partial_x^2 + V$ on $(-2, 2)$. The solution of the corresponding initial boundary value problem (1.1) is $\psi(x, t) = \psi_0(x)\exp(-ik_*^2 t)$, where k_* is a real root of the function $f(k) := \sqrt{V_* - k^2} - k\tan(k)\tanh(\sqrt{V_* - k^2})$.

In Fig.1 we plot the DG norm of the Galerkin error obtained for $V_* = 20$ and a sequence of space–time, uniform, Cartesian meshes.

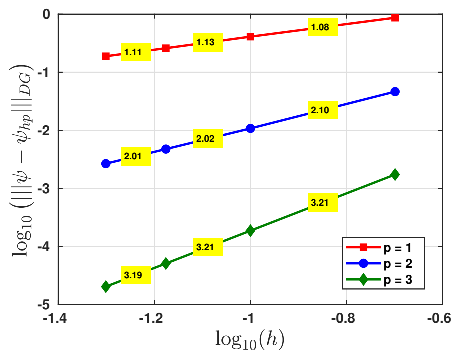

Figure 1: Trefftz-DG error for $V_* = 20$ and $k_* \approx 3.7319$.

References

[1] O. Cessenat and B. Després, Application of an ultra weak variational formulation of elliptic PDEs to the two-dimensional Helmholtz problem., *SIAM J. Num. Anal.* **35(1)** (1998), pp. 255–299.

[2] S. Gómez and A. Moiola, A space–time Trefftz discontinuous Galerkin method for the linear Schrödinger equation, *SIAM J. Num. Anal.* **60(2)** (2022), pp. 688–714.