Trefftz Approximations in Complex Media: Accuracy and Applications

Igor Tsukerman
Department of Electrical and Computer Engineering, The University of Akron
Akron, OH 44325-3904, USA
igor@uakron.edu

Shampy Mansha, Y. D. Chong
School of Physical & Mathematical Sciences, Nanyang Technological University
21 Nanyang Link, Singapore 637371
yidong@ntu.edu.sg

Vadim A. Markel
Department of Radiology, University of Pennsylvania, Philadelphia, PA 19104, USA
vmarkel@pennmedicine.upenn.edu

Abstract

Approximations by Trefftz functions are rapidly gaining popularity in the numerical solution of boundary value problems of mathematical physics. By definition, these functions satisfy locally, in weak form, the underlying differential equations of the problem, which often results in high-order or even exponential convergence with respect to the size of the basis set. We highlight two separate examples of that in applied electromagnetics and photonics: (i) homogenization of periodic structures, and (ii) numerical simulation of electromagnetic waves in slab geometries. Extensive numerical evidence and theoretical considerations show that Trefftz approximations can be applied much more broadly than is traditionally done: they are effective not only in physically homogeneous regions but also in complex inhomogeneous ones. Two mechanisms underlying the high accuracy of Trefftz approximations in such complex cases are pointed out. The first one is related to trigonometric interpolation and the second one – somewhat surprisingly – to well-posedness of random matrices.

Keywords: Trefftz approximations, convergence, Maxwell’s equations, homogenization, photonic devices, wave scattering, interpolation, finite difference schemes, random matrices

2010 MSC: 65M06, 76M20, 35B27, 76M50, 74Q15, 35Q61, 15B52

1Corresponding author.

Preprint submitted to Computers & Mathematics with Applications January 30, 2018
1. Introduction

Many classical numerical methods for partial differential equations rely on polynomial or piecewise-polynomial approximations of the solution. Examples include traditional finite difference (FD) schemes, the finite element method (FEM), and the boundary element method (BEM). But a strong incentive to achieve qualitatively higher accuracy of the numerical solution has led, over several decades of research, to the development of Trefftz-based methods. By definition, Trefftz functions satisfy locally (in weak form) the underlying differential equations of the problem, which often results in high-order algebraic or even exponential convergence with respect to the dimension of the basis. This qualitative accuracy improvement has been demonstrated in a large variety of mathematical methods and engineering applications: Domain Decomposition [1, 2], Generalized FEM [3, 4, 5, 6, 7, 8], Discontinuous Galerkin [2, 9, 10, 11, 12, 13, 14, 15], and finite difference (“Flexible Local Approximation Methods,” FLAME) [16, 17, 18, 19].

It is not our intention to review all, or even some, of these Trefftz function-oriented methods; a few good reviews are already available: [20, 21] and especially [22]. Rather, our focus is on one question central in these methods: why are Trefftz approximations so effective?

A simplified intuitive picture is shown in Fig. 1, left panel. Several incident waves, schematically indicated with solid arrows, are impinging on an object (in general, inhomogeneous) and give rise to the respective total fields inside and to scattered field outside that object. (For visual clarity, only the incident waves are sketched in the figure, and their number is limited to three.) The total fields inside the scatterer, by definition, form a Trefftz set which can be used to approximate the field induced by another wave, indicated with a dashed arrow and a question mark in Fig. 1. This approximation of one physically meaningful solution by other physically meaningful solutions (as opposed to, say, generic polynomials) certainly makes intuitive sense but is not trivial from the mathematical perspective.

The right panel of Fig. 1 illustrates a more interesting, and more complicated, case. Suppose that the original inhomogeneous scatterer is fixed, but there may be additional objects (such as S1, S2, S3) in the computational domain; moreover, each Trefftz function may correspond to different objects being present. For example, the first Trefftz function (e.g. the one indicated with the black arrow for the incoming wave) might correspond to only one additional object being present (e.g. S1), while the second Trefftz function (blue arrow) might correspond to S1, S2 and S3 being present, etc.; whereas in the case of the unknown field (dashed arrow) only the main scatterer and no additional objects might be there. Obviously, under such conditions, little can be inferred about the unknown solution from the Trefftz basis in the whole domain. However, the field within any small subdomain \( \Omega_h \) inside the original scatterer can – somewhat surprisingly and under non-restrictive assumptions – still be accurately approximated with a superposition of the known Trefftz waves. This is the central issue of Sections 6.2, 6.3.
Figure 1: Several incident waves (schematically indicated with solid arrows) give rise to the respective total fields inside an inhomogeneous scatterer. These total fields, by definition, form a Trefftz set. This Trefftz set can be used to approximate the field induced by another wave, indicated with a dashed arrow and a question mark. For visual clarity, only three Trefftz waves are sketched, and only the incident components. Left: one inhomogeneous object is present. Right: one or more additional scatterers (S1, S2, S3) may or may not be present in various cases, while an approximation of the field within a given small subdomain $\Omega_h$ is sought.

The overall motivation for the paper is to highlight applications of Trefftz functions to problems involving complex, inhomogeneous media. Much of mathematical analysis so far has revolved around the homogeneous case (that is, equations with constant coefficients), where cylindrical, spherical or plane waves serve as Trefftz functions for the Helmholtz equation, while harmonic polynomials are used for the Laplace equation. One can refer, for example, to papers by Melenk, Hiptmaier, Moiola, Perugia et al. cited above, to the references in these papers, and to Perrey-Debain’s paper [23]. Much less attention has been paid to the inhomogeneous case [24, 25], which is substantially more complicated but at the same time more rewarding in practice.

For illustration, in Sections 4 and 5 we consider two application examples where Trefftz approximations prove to be effective for two different variations of the generic setup shown in Fig. 1. The first example is non-asymptotic and nonlocal two-scale homogenization. Instead of a single scatterer, one deals in this case with a periodic structure; Trefftz functions on the fine scale are Bloch waves traveling in different directions, and on the coarse scale – the corresponding plane waves.

The second example involves a common setup in silicon photonics: a patterned finite-thickness slab. This problem is especially challenging computationally when the pattern is non-periodic and the slab is geometrically large relative to the vacuum wavelength. One possible simulation procedure relies on high-order Trefftz difference schemes (FLAME). The Trefftz bases are computed “locally,” i.e. over relatively small segments of the structure (Section 5).

Sections 2 and 3 provide background information needed in the application examples of Sections 4 and 5. The underlying mechanisms for the accuracy of Trefftz approximations are discussed in Section 6.
2. Preliminaries: Trigonometric Projection and Interpolation

Trigonometric approximation of periodic functions is a well-established subject. Here we summarize the key mathematical results that will be needed in Section 6.1.

For any Lipschitz-continuous periodic function \( g \) on \([-\pi, \pi]\), we consider its best possible approximation by a trigonometric polynomial \( T_n \) in the maximum norm:

\[
E_T^n(g) = \min_{\alpha, \beta} \max_{\phi \in [-\pi, \pi]} |g(\phi) - T_n(\alpha, \beta, \phi)|,
\]

where

\[
T_n(\alpha, \beta, \phi) \equiv \alpha_0 + \sum_{\nu=1}^{n} (\alpha_\nu \cos \nu \phi + \beta_\nu \sin \nu \phi),
\]

\[
\alpha \equiv \{\alpha_0, \alpha_1, \ldots, \alpha_n\}, \quad \beta \equiv \{\beta_1, \ldots, \beta_n\}
\]

A slightly modified notation of [26] is used here. Note that the total number of coefficients \( \alpha, \beta \) in the trigonometric series is \( N = 2n + 1 \).

It follows from Jackson’s theorem [27], or Theorem 41 in [26], that if the derivative \( g^{(l+1)}(\phi) \) exists and is bounded, i.e.,

\[
\left| g^{(l+1)}(\phi) \right| \leq M_{l+1}, \quad l = 0, 1, \ldots
\]

then

\[
E_T^n(g) \leq \frac{c^{l+1}M_{l+1}}{n^{l+1}}, \quad c = 1 + \frac{\pi^2}{2}
\]

For reasons that will become apparent in Section 6.1, we are interested primarily in trigonometric interpolation rather than the best approximation, and thus need to relate the two. The interpolant \( \tilde{T}_N(\phi) \) of a given function \( g(\phi) \) over a set of \( N = 2n + 1 \) equidistant knots \( \{\phi_m\} \) is defined in a standard way, by requiring that

\[
\tilde{T}_N(g, \phi_m) = g(\phi_m), \quad m = 0, 1, \ldots, N - 1
\]

\[
\phi_m = \frac{2\pi m}{N}, \quad m = 0, 1, \ldots, N - 1
\]

It is known that this interpolant exists and is unique. Furthermore, there is an upper bound for the interpolation error:

\[
\|g - \tilde{T}_N(g)\| \leq (1 + \Lambda_N)\|g - T_N\| \equiv (1 + \Lambda_N)E_T^n(g)
\]

where the infinity-norm is implied. \( \Lambda_N \) is the Lebesgue constant which itself has an upper bound [28]

\[
\Lambda_N \leq 2\pi^{-1} \log N + \frac{5}{3}
\]

All of the above information can be found in a variety of sources, including very recent ones [29, 30], Section 7 of [31].
Combining (7), (8), and (4), one has

$$\|g - \tilde{T}_N(g)\| \leq \left(2\pi^{-1} \log N + \frac{8}{3}\right) \left(1 + \frac{\pi^2}{2}\right)^{l+1} \frac{M_{l+1}}{n^{l+1}}$$  \hspace{1cm} (9)

This indicates fast uniform algebraic convergence of the interpolant with respect to the number of knots. Moreover, under additional assumptions of analyticity of \(g(\theta)\) in a strip of the complex plane \(\text{Re} \theta \in (0, 2\pi), |\text{Im} \theta| < \delta\), convergence becomes exponential (eq. (7.19) in [31]):

$$\|g - \tilde{T}_N(g)\| \leq \frac{4M \exp[-\delta(N + 1)/2]}{1 - \exp(-\delta)}$$  \hspace{1cm} (10)

We are also interested in the approximation of the integral

$$I = \int_0^{2\pi} g(\theta) \, d\theta$$  \hspace{1cm} (11)

using the values of \(g\) at the equispaced knots:

$$I_N = \frac{2\pi}{N} \sum_{m=1}^{N-1} g(\theta_m), \quad \theta_m = \frac{2\pi m}{N}$$  \hspace{1cm} (12)

(this is the trapezoidal rule for the numerical quadrature). Under the same analyticity assumptions as above, the error of this quadrature can be bounded as (eq. (7.20) in [31]):

$$\|I_N - I\| \leq \frac{8\pi M \exp[-\delta(N + 1)/2]}{1 - \exp(-\delta)}$$  \hspace{1cm} (13)

A similar result can be found in [29]; Theorem 1 there, adapted to our needs and notation, states:

If \(f\) is \(l\) times continuously differentiable and \(f^{(l)}\) is Lipschitz continuous, then

$$|I - \tilde{I}_N|, \|f - \tilde{f}_N\| = \mathcal{O}(N^{-(l+1)}).$$  \hspace{1cm} (14)

If \(f\) can be analytically continued to a \(2\pi\)-periodic function for \(-\delta < \text{Im} x < \delta\) for some \(\delta > 0\), then for any \(\hat{\delta} < \delta\),

$$|I - \tilde{I}_N|, \|f - \tilde{f}_N\| = \mathcal{O}(\exp(-\hat{\delta}N)).$$  \hspace{1cm} (15)

The qualitative conclusion of this section is that **trigonometric interpolation of a smooth periodic function provides a very accurate approximation of this function and its integrals.**
3. Preliminaries: Finite Difference Trefftz Schemes

Another preliminary subject, which will be needed in Section 5, is finite difference (FD) schemes based on Trefftz approximations – the Flexible Local approximation MEthod (FLAME) \[16, 17, 18, 19, 32, 33\]. Recall that classical FD schemes are typically derived from Taylor expansions; but this is problematic if the solution is not sufficiently smooth – e.g. at material interfaces. That is the root cause of the notorious “staircase” effect at off-grid interface boundaries. FLAME replaces Taylor polynomials with Trefftz functions, which often produces high-order schemes.

The key ideas of FLAME are as follows. Let a boundary value problem be defined in a computational domain $\Omega$ and consider a small subdomain $\Omega_h$ containing a grid “molecule” – a set of $n$ geometric entities such as grid nodes — on which the difference scheme is to be formed. Introduce also a set of $m$ degrees of freedom (DoF), also defined over $\Omega_h$. These DoF are, by definition, linear functionals, $l_\beta(u)$ ($\beta = 1, 2, \ldots, m$), each mapping any admissible field $u$ to a number (real or complex, depending on the problem). The simplest example of DoF, if $u$ is a scalar field, is the nodal values $l_\beta(u) \equiv u(r_\beta)$, where $r_1, \ldots, r_m$ are a set of grid nodes in $\Omega_h$. One may also consider fluxes, circulations, etc. as other examples of DoF in the case of vector fields.

Locally, within $\Omega_h$, the solution $u$ is approximated by a linear combination of Trefftz functions $\psi_\alpha$ ($\alpha = 1, 2, \ldots, n$): $u(r) \approx u_h(r) \equiv \sum_\alpha c_\alpha \psi_\alpha(r) = \bar{c}^T \bar{\psi}(r)$, \hspace{1cm} (16)
where $\bar{c} \in \mathbb{C}^n$ is a coefficient vector and $\bar{\psi}$ is a vector of basis functions (both generally complex). For each patch (i.e. for each grid “molecule”) we seek an FD equation of the form $m \sum_{\beta=1} s_\beta l_\beta(u) = 0$, \hspace{1cm} (17)
where $\bar{s} = (s_1, s_2, \ldots, s_m)^T$ is a vector of complex coefficients (a “scheme”) to be determined. In the simplest version of FLAME, the scheme is required to be exact for any linear combination (16) of basis functions. Then, after straightforward algebra, one obtains \[17, 18\]
\[ \bar{s} \in \text{Null}(N^T), \quad \text{where} \quad N^T_{\alpha\beta} = l_\beta(\psi_\alpha). \] \hspace{1cm} (18)
There are also least-squares versions of this idea \[34, 16\].

Many illustrative examples are given in \[32, 17, 18\]. Here we mention just one of them, closely related to the construction of FLAME schemes in Section 5. For the 2D Helmholtz equation, one may consider a Trefftz basis set of eight plane waves traveling at angles $\phi_0 + m\pi/4$ ($m = 0, 1, \ldots, 7$), where $\phi_0$ is a given angle; practical choices are $\phi_0 = 0$ or $\phi_0 = \pi/8$. Evaluating these plane waves over a standard $3 \times 3$ grid “molecule,” one obtains an $8 \times 9$ matrix $N^T$ whose null vector is the FLAME scheme. The result for $\phi_0 = 0$ is a nine-point ($3 \times 3$) order-six scheme \[18\]. For $\phi_0 = \pi/8$, one arrives at a scheme derived by Babuska et al in 1995 \[35\] from very different considerations.
4. Trefftz Homogenization of Electromagnetic Structures

We consider Trefftz-based homogenization of electromagnetic periodic structures (photonic crystals and metamaterials). The general description of the problem in this section follows [36, 37] closely, but our focus here is on Trefftz approximation, the importance of other aspects of the problem notwithstanding.

The physical essence of the problem is as follows. A sample of a periodic material (for simplicity, a finite-thickness slab) is illuminated by incoming monochromatic electromagnetic waves at a given frequency \( \omega \) and the corresponding free-space wavenumber \( k_0 = \omega/c \). The periodic medium in the sample is to be replaced with a homogeneous material in such a way that the scattering wave pattern would be preserved as accurately as possible.

Following [36, 37], let us define the problem more precisely. Assume that the intrinsic dielectric permittivity \( \varepsilon(r) \) within the slab is lattice-periodic, and that all material constituents are nonmagnetic, \( \mu(r) = 1 \). Let all constitutive relationships be local and linear, and let the sample be illuminated by monochromatic waves with a given far-field pattern; these waves are reflected by the metamaterial.

The problem has two principal scales (levels). Fine-level fields are the exact solutions of Maxwell’s equations for given illumination conditions for a given sample. These fields are denoted with small letters \( e, d, h \) and \( b \). In general, their variation in space is rapid and consistent with the microstructure of metamaterial cells. Coarse-level fields \( E, D, H, B \) vary on a characteristic scale greater than the cell size. They represent some smoothed (averaged) versions of the fine-level fields and are auxiliary mathematical constructions rather than measurable physical quantities. The coarse-level fields are sought to satisfy Maxwell’s equations and all interface boundary conditions as accurately as possible.

Importantly, effective magnetic properties of metamaterials cannot be determined from the bulk behavior alone as a matter of principle. This is due, in particular, to the fact that the Maxwell equation \( \nabla \times H = -ik_0D \) is invariant with respect to an arbitrary simultaneous rescaling of vectors \( H \) and \( D \). Loosely speaking, bulk behavior defines the dispersion relation only, while magnetic characteristics depend on the boundary impedance as well.

We assume that a periodic composite (a photonic crystal) is contained between the planes \( z = 0 \) and \( z = L \); this eliminates the difficult consideration of field behavior near corners. The fine-level fields satisfy macroscopic Maxwell’s equations of the form

\[
\nabla \times h(r) = -ik_0 \varepsilon(r)e(r), \quad \nabla \times e(r) = ik_0 h(r) \tag{19}
\]

everywhere in space, supplemented by the usual radiation boundary conditions at infinity. Outside of the slab, the most general solution to (19) can be written as a superposition of incident, transmitted and reflected waves. For the electric
field, we can write these in the form of angular-spectrum expansions [37]:

\[ e_i(r) = \int s_i(k_x, k_y) e^{i(k_x x + k_y y + k_z z)} \, dk_x dk_y , \quad (20a) \]

\[ e_t(r) = \int s_t(k_x, k_y) e^{i(k_x x + k_y y + k_z z)} \, dk_x dk_y , \quad z > L , \quad (20b) \]

\[ e_r(r) = \int s_r(k_x, k_y) e^{i(k_x x + k_y y - k_z z)} \, dk_x dk_y , \quad z < 0 , \quad (20c) \]

where

\[ k_z = \sqrt{k_0^2 - k_x^2 - k_y^2} , \quad (21) \]

and the square root branch is defined by the condition \( 0 \leq \arg(k_z) < \pi \). Expressions for the magnetic field are obtained from (20) by using the second Maxwell equation in (19). In (20), \( s_i(k_x, k_y) \), \( s_t(k_x, k_y) \) and \( s_r(k_x, k_y) \) are the angular spectra of the incident, transmitted and reflected fields. Waves included in these expansions can be both evanescent and propagating. For propagating waves, \( k_x^2 + k_y^2 < k_0^2 \), otherwise the waves are evanescent.

Everywhere in space, the total electric field \( e(r) \) can be written as a superposition of the incident and scattered fields, viz,

\[ e(r) = e_i(r) + e_s(r) . \quad (22) \]

Outside of the material, the reflected and transmitted fields form the scattered field:

\[ e_s(r) = \begin{cases} e_r(r), & z < 0 , \\ e_t(r), & z > L . \end{cases} \quad (23) \]

The scattered field inside the material is also formally defined by (22).

It is natural to approximate fine-level fields via a basis set of Bloch waves traveling in different directions:

\[ e_{m\alpha}(r) = \tilde{e}_{m\alpha}(r) \exp(iq_{m\alpha} \cdot r) , \quad h_{m\alpha} = \tilde{h}_{m\alpha}(r) \exp(iq_{m\alpha} \cdot r) , \quad (24) \]

where index \( \alpha \) labels both the wave vector and the polarization state of the Bloch wave in a lattice cell \( m \); \( \tilde{e}_{m\alpha}(r), \tilde{\mathbf{h}}_{m\alpha}(r) \) are the respective lattice-periodic factors. As the notation indicates, the basis is defined cell-wise; different bases in different lattice cells could be used. This makes the homogenization problem tractable and reducible to a single cell, rather than global and encompassing the whole sample.

On the coarse scale, a natural counterpart of the fine-scale Bloch basis is a set of generalized plane waves

\[ \Psi_{m\alpha} = \{ E_{m\alpha}, H_{m\alpha} \} = \{ E_{0m\alpha}, H_{0m\alpha} \} \exp(iq_{m\alpha} \cdot r) \quad (25) \]

which satisfy Maxwell’s equations in a homogeneous but possibly anisotropic medium; subscript ‘0’ indicates the field amplitudes to be determined.

Further technical details of the procedure can be found in [37, 36]. The final result is as follows. First, the coarse-level wave vector for each plane wave is
taken to be the same as its counterpart for the corresponding Bloch wave, which is already reflected in our notation above (24), (25). Secondly, the amplitudes \( \{ E_{0m\alpha}, H_{0m\alpha} \} \) of each plane wave as the boundary average of the tangential components of the respective fine-scale Bloch wave:

\[
E_{0m\alpha} = A_{m}^{\tau} \hat{e}_{m\alpha}, \quad H_{0m\alpha} = A_{m}^{\tau} \hat{h}_{m\alpha}
\]

(26)

The averaging operator \( A_{m}^{\tau} \) for tangential components of a generic vector field \( \mathbf{f} \), and a similar operator \( A_{m}^{n} \) for normal components, are defined, in the case of an orthorhombic cell \( C_{m} \), as follows:

\[
(A_{m}^{\tau})_{\gamma} \mathbf{f} \equiv \frac{\int_{\partial C_{m}} f_{\gamma} |\hat{n} \times \hat{r}_{\gamma}| dS}{\int_{\partial C_{m}} |\hat{n} \times \hat{r}_{\gamma}| dS}, \quad \gamma = 1, 2, 3; \quad \hat{r}_{1,2,3} = \hat{x}, \hat{y}, \hat{z}
\]

(27)

\[
(A_{m}^{n})_{\gamma} \mathbf{f} \equiv \frac{\int_{\partial C_{m}} f_{\gamma} |\hat{n} \cdot \hat{r}_{\gamma}| dS}{\int_{\partial C_{m}} |\hat{n} \cdot \hat{r}_{\gamma}| dS}
\]

(28)

(here \( |\hat{n} \times \hat{r}_{\gamma}| \) and \( |\hat{n} \cdot \hat{r}_{\gamma}| \) act simply as Kronecker deltas for the faces of the cell parallel or perpendicular to a given coordinate direction \( \hat{r}_{\gamma} \), \( \gamma = 1, 2, 3 \).) Note that the averages in (26) involve the periodic factor of the Bloch wave.

The amplitudes \( E_{0m\alpha}, H_{0m\alpha} \), along with the Bloch wave vector, define the coarse-level basis function \( \alpha \) in a lattice cell \( m \).

The homogenization procedure of [36, 37] leads to a system of algebraic equations of the form

\[
\Psi_{DB}^{\text{I.S.}} = \mathcal{M} \Psi_{EH}
\]

(29)

Here ‘I.S.’ stands for ‘least squares’. Each column of the rectangular matrix \( \Psi_{EH} \) corresponds to a given coarse-level basis function \( \alpha \), and the entries of that column are the \( xyz \)-components of the wave amplitudes \( E_{0m\alpha}, H_{0m\alpha} \). The number of columns \( n \) is equal to the chosen number of basis functions; the number of rows is, in general, six, unless some of the field components are known to be zero (e.g. for \( s \)- or \( p \)-polarized waves). The \( \Psi_{DB} \) matrix is completely analogous and contains the DB amplitudes derived from Maxwell’s curl equations:

\[
B_{0m\alpha} = k_{0}^{-1} q_{ma} \times E_{0m\alpha}, \quad D_{0m\alpha} = -k_{0}^{-1} q_{ma} \times H_{0m\alpha}
\]

(30)

The (local) material tensor is represented, in general, by a \( 6 \times 6 \) matrix. Since the number of columns in matrix \( \Psi_{EH} \) is typically greater than the number of rows, the matrix equation (29) for the material tensor is solved in the least squares sense:

\[
\mathcal{M} = \Psi_{DB}^{\dagger} \Psi_{EH}^{\dagger}; \quad \delta_{\text{I.S.}} = ||\Psi_{DB} - \mathcal{M} \Psi_{EH}||_{2}
\]

(31)

where \( \Psi_{EH}^{\dagger} \) is the Moore-Penrose pseudoinverse of \( \Psi_{EH} \), \( \delta_{\text{I.S.}} \) is the associated least-squares error.
Figure 2: Example A of a layered medium from [38, 37]. The real part of $R$ (left) and $T$ (right) vs. the sine of the angle of incidence; non-asymptotic and nonlocal homogenization. The lattice cell contains three layers of widths $a/4$, $a/2$ and $a/4$, with scalar permittivities $\epsilon_1$, $\epsilon_2$, and $\epsilon_3$, respectively. ($\epsilon_1 = 4 + 0.1i$ and $\epsilon_2 = 1$.) Fine-level basis: $2n_{\text{dir}}$ Bloch modes traveling at $n_{\text{dir}} = 7$ different angles in $(-\pi/2, \pi/2)$; $n_{\text{dir}} = 7$. The kernel width parameter $\tau_0 = a$. The reflection and transmission coefficients from nonlocal homogenization are visually indistinguishable from the exact ones. (The nonlocal procedure includes two additional DoF: the convolution integrals of the tangential components of the electric and magnetic fields.)
Figure 3: Example A of a layered medium from [38, 37]. Absolute error in $R$ (left) and $T$ (right) vs. $a/\lambda$; non-asymptotic and nonlocal homogenization. The lattice cell contains three layers of widths $a/4$, $a/2$ and $a/4$, with scalar permittivities $\epsilon_1$, $\epsilon_2$, and $\epsilon_3$, respectively. ($\epsilon_1 = 4 + 0.1i$ and $\epsilon_2 = 1.$) Fine-level basis: $2n_{\text{dir}}$ Bloch modes traveling at $n_{\text{dir}} = 7$ different angles in $(-\pi/2, \pi/2)$; $n_{\text{dir}} = 7$. The kernel width parameter $\tau_0 = a$. The accuracy of the nonlocal procedure is, by far, the highest. (The nonlocal procedure includes two additional DoF: the convolution integrals of the tangential components of the electric and magnetic fields.)
As demonstrated in [36], the homogenization accuracy can be further improved by including, in addition to the $EH$ amplitudes, integral DoF of the form

$$D(r) = \int_{\Omega} \mathcal{E}(r, r') E(r') \, d\Omega$$  \hspace{1cm} (32)

where $\mathcal{E}$ is a convolution kernel depending only on the coordinates tangential to the boundary of the sample:

$$\mathcal{E}(r, r') = \mathcal{E}(\hat{n} \times r, \hat{n} \times r')$$

A natural (but certainly not unique) choice for this kernel is a Gaussian

$$\mathcal{E}(r, r') = \mathcal{E}_0 \exp(-\tau_0^{-2} |\hat{n} \times (r - r')|^2)$$

where the amplitude $\mathcal{E}_0$ and width $\tau_0$ are adjustable parameters, and $\hat{n}$ is the unit normal vector.

Since our focus is on the approximation properties of Trefftz functions and not on the homogenization procedure per se, we do not discuss the physics of the problem here, or the merits and demerits of nonlocal vs. local theory.\footnote{It should, however, be noted that our nonlocal procedure operates in real space, in contrast with $k$-space techniques that we critiqued elsewhere [38].} We also omit further technical details and limit ourselves to just one illustration example.

Shown in Figs. 2 and 3 are the reflection $R$ and transmission $T$ coefficients for electromagnetic waves propagating through a layered slab. (These coefficients are defined in a standard way, as the ratio of the complex amplitudes of the reflected/transmitted waves to that of the incident wave.) The geometric and physical parameters correspond to Example A of [38]: the lattice cell of a width $a$ contains three layers of widths $a/4$, $a/2$ and $a/4$, with scalar permittivities $\epsilon_1$, $\epsilon_2$, and $\epsilon_3$, respectively; $\epsilon_1 = 4 + 0.1i$ and $\epsilon_2 = 1$. The fine-level Trefftz basis contains $2n_{\text{dir}}$ Bloch modes traveling at $n_{\text{dir}} = 7$ equispaced angles in $(-\pi/2, \pi/2)$; $n_{\text{dir}} = 7$. In nonlocal homogenization, the additional DoF are the integrals of the form (32), with the Gaussian kernel of width $\tau_0 = a$.

Fig. 2 shows the real part of $R$ and $T$ as a function of the angle of incidence, for $a/\lambda = 0.2$. (The imaginary parts are not plotted to save space but are qualitatively similar). Since analytical solutions for wave propagation in layered media are fairly simple and well known, one may easily calculate the errors in $R$ and $T$; those are plotted in Fig. 3.

The figures show that our numerical results, especially for nonlocal homogenization, are highly accurate. In fact, we are not aware of any alternative methods that could produce a comparable level of accuracy at a comparable computational cost.\footnote{The latter provision is needed to exclude from consideration “brute force” numerical optimization of the material tensor.}

What explains this high accuracy? Plausible mechanisms are presented in Section 6.
5. Electromagnetic Waves in Slab Geometry

5.1. Formulation of the problem

The general description of the problem in this section closely follows the recently published paper [39], which explores a new computational method, “FLAME-slab,” for electromagnetic wave scattering problems in aperiodic photonic structures – specifically, structures possessing short-range regularity but lacking long-range order, such as amorphous or quasicrystalline lattices. Structures of this type can exhibit a variety of interesting properties, e.g. highly isotropic band gaps and fractal photonic spectra, but are difficult to study numerically \[40, 41, 42, 43, 44, 45, 46, 47, 48, 49\]. FLAME-slab exploits the short-range regularity of the structure by generating a Trefftz basis in a relatively small segment of the structure.

As an example, we consider a slab substrate patterned with aperiodically placed but geometrically identical pillars (Fig. 4). The slab has thickness \(d\), and there are 10 pillars of height \(d\) and width \(w = 0.8d\). Both the substrate and the pillars have dielectric constant \(\varepsilon = 12\). The surrounding medium is air. In our calculations, we adopt computational units where the vacuum constants and the speed of light are all set to unity: \(\varepsilon_0 = 1, \mu_0 = 1, c = 1\). Then the frequency \(f\) has the units of \(1/\lambda\) (where \(\lambda\) is the free space wavelength).

Light is incident from the top, as shown in Fig. 4, with a wavenumber \(k\) and incidence angle \(\theta_{inc}\) relative to the \(z\)-axis. We take the entire structure to be a supercell of length \(L_x\), with quasi-periodic boundary conditions (see below). The electric and magnetic fields in the structure are governed by Maxwell’s equations:

\[
\nabla \times \mathbf{E} = ik \mathbf{H}, \quad \nabla \times \mathbf{H} = -ik\varepsilon \mathbf{E}.
\]

Figure 4: Schematic for the structure used in our calculation. The structure consists of 10 dielectric pillars positioned aperiodically on a dielectric slab. Light is incident from the top, with wavenumber \(k\) and incidence angle \(\theta_{inc}\).
We consider the case where the electric field is $s$-polarized, $\mathbf{E} = E\hat{y}$, so that the magnetic field has the form $\mathbf{H} = H_x\hat{x} + H_z\hat{z}$. The quasi-periodic boundary conditions are:

$$
\begin{align*}
\mathbf{E}(L_x/2, z) &= \mathbf{E}(-L_x/2, z) \exp(ik_x L_x), \\
\mathbf{H}(L_x/2, z) &= \mathbf{H}(-L_x/2, z) \exp(ik_x L_x),
\end{align*}
$$

(34)

where $k_x = k \sin \theta_{\text{inc}}$ is the $x$-component of the incident wave vector $k$.

The scattered electric field is defined as

$$
E_{\text{scat}}(\mathbf{r}) = E_{\text{total}}(\mathbf{r}) - E_{\text{inc}}(\mathbf{r}), 
$$

(35)

where $E_{\text{total}}$ and $E_{\text{inc}}$ are the total and incident electric fields respectively. The magnetic field is split similarly. The scattered field is purely outgoing on both the upper side (towards the negative $z$-direction) and the lower side (towards the positive $z$-direction) of the structure.

Fig. 5(a) shows the discretization scheme for FLAME. The structure is discretized into $N_x$ grid points in the horizontal direction. In the vertical direction, the number of layers is deliberately limited to three ($z_-, z_0, z_+$), to demonstrate that FLAME-slab can work well on very coarse grids. The electric fields in these three layers are denoted with $E_\alpha^\Gamma$, $\alpha = \{-, 0, +\}$. Similarly, the magnetic fields in the upper and bottom layers are denoted with $H_\beta^\Gamma$, $\beta = \{-, +\}$.

We define three distinct types of patches, with their corresponding grid “molecules” and FD stencils. The first is a standard 9-point stencil containing just the electric field degrees of freedom (DoF), as shown in the left panel of Fig. 5(b). The second is a 6-point stencil over the middle and top layers, containing both the electric and magnetic fields (middle panel). The third is a 6-point stencil over the middle and bottom layers, containing both the electric and magnetic fields (right panel of Fig. 5(b)).

Each type of patch thus contains 9 degrees of freedom. FLAME uses 8 basis functions, to be determined by solving Maxwell’s equations for “Trefftz cells” matching the local dielectric environment in each patch. Each Trefftz cell contains a segment of length $L_i$ with a single pillar on the substrate; quasi-periodic boundary conditions are imposed. We choose $L_i \ll L_x$, so that Maxwell’s equations can be solved much more rapidly for the Trefftz cell than for the entire aperiodic structure. We generate 8 different Trefftz basis functions by picking two different segment lengths ($L_1$ and $L_2$), and four different angles of incidence for each $L_i$. To compute the fields in the Trefftz cell, we use the existing rigorous coupled wave analysis (RCWA) solver $S^4$ [50].

The FLAME procedure now yields a matrix equation of the form

$$
\mathbf{A}_{\text{FLAME}} \psi_{\text{tot}} = 0,
$$

(36)

where $\mathbf{A}_{\text{FLAME}}$ is a matrix of stencil coefficients and $\psi_{\text{tot}}$ is a column vector containing the nodal values of the total electric and magnetic fields. For the present choice of discretization, $\mathbf{A}_{\text{FLAME}}$ has size $3N_x \times 5N_x$, and $\psi_{\text{tot}}$ has size $5N_x \times 1$; we emphasize that this is just one possible choice of discretization,
Figure 5: (a) Discretization of the structure into $N_x \times 3$ nodes ($N_x$ in the horizontal direction and 3 layers in the vertical direction). (b) The 9 point stencil patch (in (a)) subdivided into patches: Left: subpatch containing 9 nodes with single DOF where the electric fields are determined, the right and central subpatch: having 6 nodes where 3 nodes with double circles have double DoF to determine the magnetic fields.
and other choices can be handled in a straightforward way. Details about the calculation of $A_{\text{FLAME}}$ can be found in Ref. [39].

FLAME schemes need to be supplemented by radiation boundary conditions. One way of implementing such conditions is via the Dirichlet-to-Neumann (DtN) maps in the semi-infinite air strips above and below the slab. DtN maps can be efficiently calculated via Fast Fourier Transforms (FFTs). More specifically, from Maxwell’s equations in free space,

$$H_{\text{scat}}(x, z) = \frac{i}{\omega} \frac{\partial E_{\text{scat}}}{\partial z}$$ \quad (37)

where $\omega = 2\pi f = k$ is the operating frequency. We expand the scattered electric field into its Fourier series:

$$E_{\text{scat}}(x, z) = \sum_{n} c_n \exp[i(k_{nz} z + k_{nx} x)] \exp(iq x),$$ \quad (38)

where the factor of $\exp(iq x)$ comes from the quasiperiodic boundary conditions in the $x$ direction, with $q = k \sin \theta_{\text{inc}}$. The summation $n$ runs over the integer values, $k_{nx} = 2\pi n/L_x$ is the horizontal wavenumber, and

$$k_{nz} = \pm \sqrt{k^2 - (k_{nx} + q)^2}.$$ \quad (39)

In the above equation, the choice of $\pm$ depends upon the layer we are dealing with ($-$ for the upper layer and $+$ for the bottom layer), so that the scattered field is outgoing. Using Eqs. (37) and (38) gives

$$H_{\text{scat}}(x, z) = -\frac{1}{\omega} \sum_{n} c_n k_{nz} \exp[i(k_{nz} z + k_{nx} x)] \exp(iq x).$$ \quad (40)

Thus, the scattered electric and magnetic fields can be related using FFTs:

$$H_{\text{scat}}(x_m, z_{\pm}) = -\frac{1}{\omega} e^{-im\pi(1-N_x^{-1})} e^{iq x_m}$$

$$\times \text{FFT}_m \left\{ k_{nz} \text{FFT}_n \left\{ E_{\text{scat}}(x_m', z_{\pm}) e^{im'\pi(1-N_x^{-1})} e^{-iq x_{m'}} \right\} \right\},$$ \quad (41)

where for $p = m, m'$,

$$x_p = -\frac{L_x}{2} + \frac{L_x p}{N_x}, \quad (p = 0, 1, \ldots, (N_x - 1)).$$ \quad (42)

We are using the FFT convention

$$\text{FFT}_m \left\{ f_n \right\} = \sum_{n=0}^{N-1} e^{-2\pi i mn/N} f_n.$$ \quad (43)

where $f_n$ is the $n$-th vector component.
Finally, we arrive at an equation of the form

\[
\begin{pmatrix}
A_{\text{FLAME}} \\
A_{\text{BC}}
\end{pmatrix}
\psi_{\text{scat}} =
\begin{pmatrix}
-A_{\text{FLAME}} \psi_{\text{inc}} \\
0
\end{pmatrix},
\]

where \(A_{\text{FLAME}}\) is a sparse sub-matrix obtained using FLAME, and \(A_{\text{BC}}\) is sub-matrix obtained from the boundary relations [39]. In our 2D examples, standard direct solvers in Matlab were sufficient for finding \(\psi_{\text{scat}}\). In 3D, iterative solvers will need to be used, but this issue is completely beyond the scope of the present paper.

5.2. Results

Fig. 6 compares the fields calculated using FLAME-slab to a reference RCWA calculation. The structure is the one shown in Fig. 4, with frequency \(f = 0.25\) and incidence angle \(\theta_{\text{inc}} = 30^\circ\). For the FLAME-slab calculation, we take a horizontal discretization of \(N_x = 101\), and precompute the Trefftz basis functions with \(N_G = 150\) (the number of expansion terms used in the RCWA subroutine [50]) and \(N_T = 800\) (the cell discretization used for storing the Trefftz basis functions). The pure RCWA reference solution is computed using \(N_G^{\text{ref}} = 1000\) – an “overkill” setting meant to produce a highly accurate solution. The figure shows two representative field components: the real part of the scattered electric field \(E_0^{\text{scat}}\) in the middle layer \((z_0)\) in Fig. 6(a), and the scattered magnetic field \(H_z^{\text{scat}}\) in the bottom layer \((z+)\) in Fig. 6(b). The FLAME-slab solution is seen to be in excellent agreement with the RCWA solution.

The central issue of this paper is approximation, and the finite-difference measure most closely related to it is the (normalized) consistency error

\[
\xi = \frac{\|A_{\text{FLAME}} \psi_{\text{ref}}^\text{total}\|}{\|A_{\text{FLAME}}\| \|\psi_{\text{ref}}^\text{total}\|},
\]

where Euclidean vector norms and the Frobenius matrix norm are implied.

In (45), \(\psi_{\text{ref}}^\text{total}\) should ideally be the exact solution, which is not available; hence an overkill RCWA solution with \(N_G^{\text{ref}} = 1000\) is used in its stead.

Since FLAME-slab contains a few adjustable parameters, we study the dependence of the consistency error on these parameters separately.

Fig. 7 displays the consistency error versus the incidence angle \(\theta_{\text{inc}}\). For this calculation, we set \(N_x = 101\), \(N_G = 150\), \(N_T = 800\) and \(f = 0.25\). The consistency error oscillates but remains bounded by \(\lesssim 10^{-5}\) over the entire range of \(\theta_{\text{inc}}\).

Fig. 8 shows the consistency error versus the vacuum wavelength \(\lambda_{\text{vac}}\) for the 10 pillar system, with fixed incidence angle \(\theta_{\text{inc}} = 30^\circ\). The FLAME-slab parameters are fixed at \(N_x = 101\), \(N_G = 150\), and \(N_T = 800\). As \(\lambda_{\text{vac}}\) is increased, \(\xi\) decreases from \(10^{-4}\) to around \(10^{-6}\). Past this point, \(\xi\) saturates.

Fig. 9 shows the consistency error versus spatial discretization \(N_x\), for \(f = 0.25\) and normal incidence \(\theta_{\text{inc}} = 0\). The other FLAME-slab parameters are \(N_G = 150\) and \(N_T = 800\). The consistency error decreases with \(N_x\), saturating at \(\approx 10^{-7}\) for \(N_x \gtrsim 500\).
Figure 6: (a) Real part the scattered electric field $E_{\text{scat}}$ in the middle layer ($z_0$). (b) Real part of the scattered magnetic field $H_{\text{scat}}$ in the bottom layer ($z_1$). The calculations were done for the slab shown in Fig. 4, with $f = 0.25$ and $\theta_{\text{inc}} = 30^\circ$. The FLAME-slab parameters are $N_x = 101, N_G = 150$, and $N_T = 800$. Blue dots show the FLAME-slab results and the red curve shows the result from RCWA obtained by setting $N_G^{\text{ref}} = 1000$. 
Figure 7: Consistency error ($\xi$) vs. angle of incidence $\theta_{inc}$ for the 10 pillar system as shown Fig. 4. The value of the parameters used are: $N_x = 101$, $N_G = 150$, $N_T = 800$ and $f = 0.25$.

Figure 8: Consistency error ($\xi$) vs. $\lambda_{vac}$ (vacuum wavelength) for the slab structure shown in Fig. 4, with $\theta_{inc} = 30^\circ$. The FLAME-slab parameters are $N_x = 101$, $N_G = 150$, and $N_T = 800$. 
For the purposes of the paper, the main qualitative conclusion of this section is that Trefftz functions, on which FLAME-slab is based, provide an accurate approximation of the electromagnetic field in a geometrically and physically complex structure.

6. The Accuracy of Trefftz Approximations

6.1. An Interpolation Argument

The numerical results for the two application examples of the previous sections show that Trefftz approximations are surprisingly effective. What explains their high accuracy?

As noted in the Introduction, in the mathematical literature this question has been studied primarily for homogeneous media (e.g., plane wave or cylindrical/spherical wave expansions) but needs to be posed much more broadly, because complex inhomogeneous media are of great theoretical and practical interest. This section is an attempt to understand the general mechanisms of high accuracy of Trefftz approximations.

In the case of Trefftz homogenization (Section 4), one can apply an interpolation argument using the summary in Section 2. Indeed, the key parameters in our homogenization methodology are the boundary averages of the Bloch fields (26). Each of these averages is, trivially, a periodic function of the angle (direction) of propagation of the respective Bloch wave and, as such, can be accurately approximated by the trigonometric interpolant over a set of equispaced knots. But such knots correspond precisely to the basis set of Bloch waves chosen in our procedure. The accuracy of this interpolation is (Section 4) $O(N^{l+1})$. 

Figure 9: Consistency error ($\xi$) vs. $N_x$ for the slab shown in Fig. 4, with $f = 0.25$ and $\theta_{inc} = 0$. The FLAME-slab parameters are $N_G = 150$ and $N_T = 800$. 

For the purposes of the paper, the main qualitative conclusion of this section is that Trefftz functions, on which FLAME-slab is based, provide an accurate approximation of the electromagnetic field in a geometrically and physically complex structure.
if the respective Bloch average is \( l \) times continuously differentiable, or, under additional analyticity assumptions, even \( O(\exp(-\alpha N)) \), where \( N \) is the size of the Bloch basis set (which is the same as the number of interpolation knots).

In our second example of wave propagation and scattering in slab geometry, the interpolation argument is not sufficient. This is because our Trefftz functions are defined over a segment of the structure, whereas the full electromagnetic problem is defined on the whole structure. Hence a more sophisticated explanation for the accuracy of Trefftz approximations in this case is needed and is provided below.

We start with a slightly more abstract physical setup than that of Fig. 1. Namely, let us assume, as before, that an inhomogeneous scatterer occupies a Lipschitz domain \( \Omega \) (solid red in Fig. 10) which is enclosed in a shell \( \bar{\Omega} \) (textured area). The material parameters within \( \Omega \) are fixed, but in \( \bar{\Omega} \) they can vary or even be random. As previously, we consider a Trefftz basis corresponding to several incident waves, and are interested in approximating the field in a small subdomain \( \Omega_h \subset \Omega \). This approximation can be used, for example, to generate a high-order difference scheme in \( \Omega_h \), as was done in Section 5.

The presence of the variable layer \( \bar{\Omega} \) makes this case peculiar and especially interesting. The following section explains why accurate local Trefftz approximations can still be expected.

### 6.2. An Auxiliary “Reference” Basis

Let us assume that in \( \Omega_h \) there is an auxiliary basis \( \zeta_\alpha (\alpha = 1, 2, ..., n_\zeta) \) that can provide an accurate approximation of a (generic) solution of the wave equation:

\[
u(r) = \sum_\alpha \gamma_\alpha \zeta_\alpha(r) + \delta(r), \quad r \in \Omega_h \quad (46)\]

\[
\| \gamma \|_2 \equiv \| \{ \gamma_\alpha \} \|_2 \leq C(\Omega_h, n_\zeta, k) \| u \|_{H^1(\Omega_h)}, \quad \| \delta \|_{H^1(\Omega_h)} \leq c(\Omega_h, n_\zeta, k) \| u \|_{H^1(\Omega_h)}
\]
Here $\delta$ is an error term, $\gamma$ is a coefficient vector, $C$ and $c$ are some generic constants, the latter being “small” in some sense (see Theorems below). In the specific example of s-wave scattering in Section 5, the unknown is the $E$-field; but here we use the “noncommittal” symbol $u$ as an indication that our analysis could be applied more broadly.

Assuming that (46) holds, one applies it to the chosen set $\psi_\zeta$ of $n_T$ Trefftz waves, and arrives at the linear transformation

$$\psi_T(r) = P^{+}_{\zeta \to T}\psi_\zeta(r) + \delta_T(r)$$

where column vectors are underlined; $P^{+}_{\zeta \to T}$ is the $n_T \times n_\zeta$ transformation matrix, and $\delta_T$ is the approximation error for the Trefftz functions in terms of the $\zeta$ set. If $n_\zeta \leq n_T$, and if matrix $P^{+}_{\zeta \to T}P^{+}_{\zeta \to T}$ is invertible, then

$$\zeta(r) = P^{+}_{\zeta \to T}\psi_T(r) + P^{+}_{\zeta \to T}\delta_T(r)$$

where ‘$+$’ indicates the Moore-Penrose pseudoinverse.

The exact solution is therefore

$$u_{\text{exact}}(r) = \gamma^T\zeta(r) = \gamma^T P^{+}_{\zeta \to T}\psi_T(r) + \gamma^T P^{+}_{\zeta \to T}\delta_T(r) + \delta_u(r)$$ (47)

where $\delta_u$ is the approximation error of the exact solution via the $\zeta$ set. Thus the smallness of the Trefftz approximation error (i.e. the last term in (47)) hinges on the smallness of the norm of the pseudoinverse $P^{+}_{\zeta \to T}$ – that is, on the inverse of its minimum singular value $\sigma_{\text{min}}$; we discuss that below.

The transformations above are schematically illustrated in Fig. 6.2. If the Trefftz basis and the solution $u_{\text{exact}}$ can be approximated via the reference basis as in (46), and if $\sigma_{\text{min}}(P)$ is bounded from below, then one can approximate $u_{\text{exact}}$ via the Trefftz basis (by following, conceptually, the two solid arrows in the sketch).

An example of this auxiliary basis is, in the case of a homogeneous domain $\Omega_h$, a set of cylindrical harmonics $\zeta_{\text{cyl}}(r, k, \theta, n) = J_n(kr) \exp(in\theta)$, $n = \ldots$
0, ±1, ±2, . . .; \( J_n \) is the Bessel function of the first kind. Detailed error analyses have been carried out by Melenk, Hiptmair, Moiola and Perugia [51, 22, 52]. For our purposes, the most convenient final results can be found in [4, 53].

**Theorem 4 in [4].** Let \( \Omega \subset \mathbb{R}^2 \) be a simply connected, bounded Lipschitz domain. Let \( \bar{\Omega} \supset\supset \Omega \) and assume that \( u \in L^2(\bar{\Omega}) \) solves the homogeneous Helmholtz equation on \( \bar{\Omega} \). Then

\[
\inf_{u_p \in V_p} \| u - u_p \|_{H^1(\Omega)} \leq C \exp(-\gamma p) \| u \|_{L^2(\bar{\Omega})}
\]  

(48)

where \( V_p \equiv \text{span}\{\zeta_{cyl}(r, k, \theta, n)\}, n = 0, 1, \ldots, p; C, \gamma \) depend only on \( \Omega, \bar{\Omega}, \) and the wavenumber \( k \).

Under the assumptions of this theorem, the presence of a “buffer region” \( \bar{\Omega} - \Omega \) ensures that high-order harmonics from the boundary of \( \bar{\Omega} \) die out sufficiently. If this assumption is not made, an alternative error estimate, dependent on the level of smoothness of the solution, reads:

**Theorem 5 in [4].** Let \( \Omega \subset \mathbb{R}^2 \) be a simply connected, bounded Lipschitz domain, star-shaped with respect to a ball. Let the exterior angle of \( \Omega \) be bounded from below by \( \lambda \pi, 0 < \lambda < 2 \). Assume that \( u \in H^s(\Omega), s > 1 \), satisfies the homogeneous Helmholtz equation. Then

\[
\inf_{u_p \in V_p} \| u - u_p \|_{H^j(\Omega)} \leq C_j \left( \frac{\ln p}{p} \right)^{\lambda(s-j)} \| u \|_{H^j(\bar{\Omega})}, \quad j = 0, 1, \ldots, [s]
\]  

(49)

Obviously, in our case \( \Omega_h \) plays the role of the generic \( \Omega \) in the estimates above. These estimates of the error term \( \delta \) in (46) are valid for the 2D Helmholtz equation in a physically homogeneous medium within \( \Omega_h \).

In the special case of a homogeneous domain \( \Omega_h \), and the Trefftz set consisting of plane waves traveling in \( n_T \) equispaced angular directions, the norm of the pseudoinverse \( P_{cyl \to PW}^+ \) can be estimated explicitly. From the Jacobi-Anger expansion, the entries of the matrix \( \hat{P} \equiv P_{cyl \to PW} \) are

\[
\hat{P}_{ml} = i^l \exp \left( -iml \frac{2\pi}{n_T} \right), \quad 0 \leq m \leq n_T - 1, \quad 0 \leq l \leq n_\zeta - 1
\]  

(50)

This matrix corresponds to a discrete Fourier transform, and its columns are easily shown to be orthogonal, so that

\[
\hat{P}^+ \hat{P} = n_T I_{n_\zeta}, \quad n_\zeta \leq n_T
\]  

(51)

where \( I_{n_\zeta} \) is the identity matrix of dimension \( n_\zeta \). It then immediately follows that

\[
\| P_{cyl \to PW}^+ \|_2 = \sigma_{\text{min}}^{-1}(P_{cyl \to PW}) = n_T^{-\frac{1}{2}}
\]  

(52)

so in this case stability of the transformation is guaranteed.

---

4There is an apparent misprint in [4]: \( H^k \) instead of \( H^s \) in the norm on the right hand side.
6.3. A Connection with Random Matrix Theory

The well-posedness of the transformation noted above is not accidental, but rather is rooted in the theory of random matrices. This theory dates back to von Neumann and Wigner \cite{54,55} and is now quite mature \cite{56,57,58,59,60}. Particularly relevant to us is the following result.

**Theorem.** (Theorem 3.3, Rudelson & Vershynin \cite{60}.) Let $A$ be an $N \times n$ random matrix whose entries are independent and identically distributed subgaussian random variables with zero mean and unit variance. Then

$$P \left( \sigma_{\min}(A) \leq \epsilon(\sqrt{N} - \sqrt{n - 1}) \right) \leq (Ce)^{N-n+1} + c^N, \quad \epsilon \geq 0$$

where $C > 0$ and $c \in (0,1)$ depend only on the subgaussian moment of the entries.

The connection of the Rudelson-Vershynin theorem with the previous subsection is straightforward:

- Our Trefftz basis can be treated as a particular realization of some random distribution (e.g. angles of incidence randomly chosen and/or random properties of the “shell” $\Omega$). A notable feature of random matrix theory is universality: only mild dependence of the spectral bounds on the distribution of the random variables. Thus no overly restrictive conditions on the Trefftz basis need to be imposed.

- Clearly, the theorem is applied with $N \equiv n_T$, $n \equiv n_\zeta$.

- The assumption that the distribution is subgaussian is satisfied, in particular, by all bounded random variables and hence is not at all restrictive.\footnote{A random variable $X$ is called subgaussian if there exists a positive constant $w$ such that $P(|X| > x) \leq 2 \exp(-x^2/w^2)$ for $x > 0$.}

- Complex bases and matrices can be decomplexified by the substitutions of the form $\psi \to (\Re \psi, \Im \psi)^T$, $P \to \begin{pmatrix} \Re P & -\Im P \\ \Im P & \Re P \end{pmatrix}$. This preserves the relevant norms and hence does not affect the spectral bounds.

- The assumption of unit variance is obviously a matter of scaling only.

- The assumption of zero mean holds for any reasonable choice of the Trefftz bases by symmetry considerations.

The theorem affirms that stability (52) of the transformation is not accidental. In fact, with a probability close to one, $\sigma_{\min}(P)$ is not small, for any reasonable choice of the Trefftz basis.

\footnote{There is an apparent misprint in [60]: $n \times n$ instead of $N \times n$.}
7. Conclusion

The key argument of this paper is that Trefftz approximations – that is, approximations by functions satisfying (locally) a given differential equation – deserve to be studied and applied more broadly than is traditionally done. Conventionally, these approximations are used in homogeneous subdomains, where the underlying differential equation has constant coefficients; this is done in various contexts (GFEM, DG, FD).

As an illustration of a much broader use of Trefftz functions, the paper reviews two disparate but representative examples: (i) non-asymptotic and nonlocal two-scale homogenization of periodic electromagnetic media, and (ii) special Trefftz FD (FLAME) schemes for wave scattering from photonic structures with slab geometry. In both cases, Trefftz approximations are applied in complex inhomogeneous domains and prove to be quite effective.

We discuss possible mechanisms engendering the high accuracy of Trefftz approximations. One such mechanism is trigonometric interpolation, which itself is known to be surprisingly accurate (in comparison with other typical forms of interpolation). Another mechanism is the availability of rapidly converging local expansions of the solution (such as, or similar to, cylindrical or spherical harmonics). There is also a curious connection of Trefftz approximations with the theory of random matrices.

It is hoped that these considerations will stimulate further mathematical research and practical applications of Trefftz-based methods.

Acknowledgment

The work of IT was supported in part by the US National Science Foundation Grants DMS-1216927 and DMS-1620112. The research of SM and YC was supported by the Singapore MOE Academic Research Fund Tier 2 Grant MOE2016-T2-1-128, the Singapore MOE Academic Research Fund Tier 2 Grant MOE2015-T2-2-008, and the Singapore MOE Academic Research Fund Tier 3 Grant MOE2016-T3-1-006. The work of VM was supported in part by the US National Science Foundation Grants DMS-1216970.

References

[1] I. Herrera, Trefftz method: A general theory, Numer. Methods Partial Differential Eq. 16 (2000) 561–580.

[2] C. Farhat, R. Tezaur, J. Toivanen, A domain decomposition method for discontinuous Galerkin discretizations of Helmholtz problems with plane waves and Lagrange multipliers, International Journal for Numerical Methods in Engineering 78 (13) (2009) 1513–1531. doi:10.1002/nme.2534.
[3] J. Melenk, I. Babuška, The partition of unity finite element method: Basic theory and applications, Comput. Methods Appl. Mech. Engrg. 139 (1996) 289–314.

[4] I. Babuška, J. Melenk, The partition of unity method, Int. J. for Numer. Meth. in Eng. 40 (4) (1997) 727–758.

[5] I. Babuška, U. Banerjee, J. E. Osborn, Generalized finite element methods – main ideas, results and perspective, International Journal of Computational Methods 1 (1) (2004) 67–103. doi:10.1142/S0219876204000083.

[6] A. Plaks, I. Tsukerman, G. Friedman, B. Yellen, Generalized Finite Element Method for magnetized nanoparticles, IEEE Trans. Magn. 39 (3) (2003) 1436–1439.

[7] L. Proekt, I. Tsukerman, Method of overlapping patches for electromagnetic computation, IEEE Trans. Magn. 38 (2) (2002) 741–744.

[8] T. Strouboulis, I. Babuška, R. Hidajat, The generalized finite element method for Helmholtz equation: Theory, computation, and open problems, Computer Methods in Applied Mechanics and Engineering 195 (37) (2006) 4711 – 4731, John H. Argyris Memorial Issue. Part I. doi: 10.1016/j.cma.2005.09.019.

[9] B. Cockburn, G. Karniadakis, C.-W. Shu, The development of discontinuous Galerkin methods, in: B. Cockburn, G.E.Karniadakis, C.-W.Shu (Eds.), Discontinuous Galerkin Methods. Theory, Computation and Applications, Vol. 11 of Lecture Notes in Comput. Sci. Engrg., Springer-Verlag, New York, 2000, pp. 3–50.

[10] D. N. Arnold, F. Brezzi, B. Cockburn, L. D. Marini, Unified analysis of discontinuous Galerkin methods for elliptic problems, SIAM J. Numer. Analysis 39 (5) (2002) 1749–1779.

[11] A. Buffa, P. Monk, Error estimates for the ultra weak variational formulation of the Helmholtz equation, M2AN, Math. Model. Numer. Anal. 42 (6) (2008) 925–940.

[12] C. J. Gittelson, R. Hiptmair, I. Perugia, Plane wave discontinuous Galerkin methods: Analysis of the h-version, ESAIM: M2AN 43 (2) (2009) 297–331. doi:10.1051/m2an/2009002.

[13] G. Gabard, P. Gamallo, T. Huttunen, A comparison of wave-based discontinuous Galerkin, ultra-weak and least-square methods for wave problems, International Journal for Numerical Methods in Engineering 85 (3) (2011) 380–402. doi:10.1002/nme.2979.

[14] R. Hiptmair, A. Moiola, I. Perugia, Plane wave discontinuous Galerkin methods for the 2d Helmholtz equation: Analysis of the p-version, SIAM Journal on Numerical Analysis 49 (1) (2011) 264–284. doi:10.1137/090761057.
[15] F. Kretzschmar, A. Moiola, I. Perugia, S. M. Schnepp, A priori error analysis of space–time Trefftz discontinuous Galerkin methods for wave problems, IMA Journal of Numerical Analysis 36 (4) (2016) 1599–1635.

[16] I. Tsukerman, Trefftz difference schemes on irregular stencils, J of Comput Phys 229 (8) (2010) 2948–2963.

[17] I. Tsukerman, Electromagnetic applications of a new finite-difference calculus, IEEE Trans. Magn. 41 (7) (2005) 2206–2225.

[18] I. Tsukerman, A class of difference schemes with flexible local approximation, J. Comput. Phys. 211 (2) (2006) 659–699.

[19] I. Tsukerman, F. Čajko, Photonic band structure computation using FLAME, IEEE Trans Magn 44 (6) (2008) 1382–1385.

[20] E. Deckers, O. Atak, L. Coox, R. D’Amico, H. Devriendt, S. Jonckheere, K. Koo, B. Pluymers, D. Vandepitte, W. Desmet, The wave based method: An overview of 15 years of research, Wave Motion 51 (4) (2014) 550 – 565, Innovations in Wave Modelling. doi:10.1016/j.wavemoti.2013.12.003.

[21] Q. Qin, Trefftz finite element method and its applications, ASME Appl. Mech. Rev. 58 (5) (2005) 316–337. doi:10.1115/1.1995716.

[22] R. Hiptmair, A. Moiola, I. Perugia, A Survey of Trefftz Methods for the Helmholtz Equation, Springer International Publishing, 2016, pp. 237–279. doi:10.1007/978-3-319-41640-3_8.

[23] E. Perrey-Debain, Plane wave decomposition in the unit disc: Convergence estimates and computational aspects, Journal of Computational and Applied Mathematics 193 (1) (2006) 140 – 156. doi:10.1016/j.cam.2005.05.027.

[24] O. Laghouache, P. Bettess, E. Perrey-Debain, J. Trevelyan, Wave interpolation finite elements for helmholtz problems with jumps in the wave speed, Computer Methods in Applied Mechanics and Engineering 194 (2) (2005) 367 – 381, Selected papers from the 11th Conference on The Mathematics of Finite Elements and Applications. doi:10.1016/j.cma.2003.12.074.

[25] L.-M. Imbert-Gérard, Interpolation properties of generalized plane waves, Numer. Math. 131 (4) (2015) 683–711. doi:10.1007/s00211-015-0704-y.

[26] G. Meinardus, Approximation of Functions: Theory and Numerical Methods, Springer, 1967.

[27] D. Jackson, The Theory of Approximation, no. v. 11 in Colloquium Publications – American Mathematical Society, Amer Mathematical Society, 1930.
[28] E. W. Cheney, T. J. Rivlin, Some polynomial approximation operators, Mathematische Zeitschrift 145 (1) (1975) 33–42. doi:10.1007/BF01214496.

[29] A. P. Austin, L. N. Trefethen, Trigonometric interpolation and quadrature in perturbed points, SIAM Journal on Numerical Analysis 55 (5) (2017) 2113–2122. doi:10.1137/16M1107760.

[30] A. P. Austin, Some new results on and applications of interpolation in numerical computation, D. Phil. Thesis (2016).

[31] L. N. Trefethen, J. A. C. Weideman, The exponentially convergent trapezoidal rule, SIAM Review 56 (3) (2014) 385–458. doi:10.1137/130932132.

[32] I. Tsukerman, Computational Methods for Nanoscale Applications: Particles, Plasmons and Waves, Springer, 2007.

[33] H. Pinheiro, J. Webb, I. Tsukerman, Flexible local approximation models for wave scattering in photonic crystal devices, IEEE Trans. Magn. 43 (4) (2007) 1321–1324. doi:0.1109/TMAG.2006.891004.

[34] A. Boag, A. Boag, R. Mittra, Y. Leviatan, A numerical absorbing boundary-condition for finite-difference and finite-element analysis of open structures, Microwave & Opt Tech Lett 7 (9) (1994) 395–398.

[35] I. Babuška, F. Ihlenburg, E. T. Paik, S. A. Sauter, A generalized finite element method for solving the Helmholtz equation in two dimensions with minimal pollution, Comput Meth Appl Mech & Eng 128 (1995) 325–359.

[36] I. Tsukerman, Classical and non-classical effective medium theories: New perspectives, Physics Letters A 381 (19) (2017) 1635 – 1640. doi:http://doi.org/10.1016/j.physleta.2017.02.028.

[37] I. Tsukerman, V. A. Markel, A nonasymptotic homogenization theory for periodic electromagnetic structures, Proc Royal Society A 470 (2014) 2014.0245. doi:10.1098/rspa.2014.0245.

[38] V. A. Markel, I. Tsukerman, Current-driven homogenization and effective medium parameters for finite samples, Phys. Rev. B 88 (2013) 125131. doi:10.1103/PhysRevB.88.125131. URL http://link.aps.org/doi/10.1103/PhysRevB.88.125131

[39] S. Mansha, I. Tsukerman, Y. Chong, The FLAME-slab method for electromagnetic wave scattering in aperiodic slabs, Optics Express 25 (2017) 32602–32617.

[40] C. Jin, X. Meng, B. Cheng, Z. Li, D. Zhang, Photonic gap in amorphous photonic materials, Phys. Rev. B 63 (2001) 195107. doi:10.1103/PhysRevB.63.195107. URL https://link.aps.org/doi/10.1103/PhysRevB.63.195107
[41] P. García, R. Sapienza, A. Blanco, C. López, Photonic glass: A novel random material for light, Advanced Materials 19 (18) (2007) 2597–2602. doi:10.1002/adma.200602426. URL http://dx.doi.org/10.1002/adma.200602426

[42] M. Florescu, S. Torquato, P. J. Steinhardt, Designer disordered materials with large, complete photonic band gaps, Proceedings of the National Academy of Sciences 106 (49) (2009) 20658–20663. doi:10.1073/pnas.0907744106. URL http://www.pnas.org/content/106/49/20658.abstract

[43] H. Noh, J.-K. Yang, S. F. Liew, M. J. Rooks, G. S. Solomon, H. Cao, Control of lasing in biomimetic structures with short-range order, Phys. Rev. Lett. 106 (2011) 183901. doi:10.1103/PhysRevLett.106.183901. URL https://link.aps.org/doi/10.1103/PhysRevLett.106.183901

[44] H. K. Liang, B. Meng, G. Liang, J. Tao, Y. Chong, Q. J. Wang, Y. Zhang, Electrically pumped mid-infrared random lasers, Advanced Materials 25 (47) (2013) 6859–6863. doi:10.1002/adma.201303122. URL http://dx.doi.org/10.1002/adma.201303122

[45] S. Mansha, Z. Yongquan, Q. J. Wang, Y. D. Chong, Optimization of tm modes for amorphous slab lasers, Opt. Express 24 (5) (2016) 4890–4898. doi:10.1364/OE.24.004890. URL http://www.opticsexpress.org/abstract.cfm?URI=oe-24-5-4890

[46] Z. Feng, X. Zhang, Y. Wang, Z.-Y. Li, B. Cheng, D.-Z. Zhang, Negative refraction and imaging using 12-fold-symmetry quasicrystals, Phys. Rev. Lett. 94 (2005) 247402. doi:10.1103/PhysRevLett.94.247402. URL https://link.aps.org/doi/10.1103/PhysRevLett.94.247402

[47] W. Steurer, D. Sutter-Widmer, Photonic and phononic quasicrystals, Journal of Physics D: Applied Physics 40 (13) (2007) R229. URL http://stacks.iop.org/0022-3727/40/i=13/a=R01

[48] S. F. Liew, S. Knitter, W. Xiong, H. Cao, Photonic crystals with topological defects, Phys. Rev. A 91 (2015) 023811. doi:10.1103/PhysRevA.91.023811. URL https://link.aps.org/doi/10.1103/PhysRevA.91.023811

[49] S. Knitter, S. F. Liew, W. Xiong, M. I. Guy, G. S. Solomon, H. Cao, Topological defect lasers, Journal of Optics 18 (1) (2016) 014005. URL http://stacks.iop.org/2040-8986/18/i=1/a=014005

[50] V. Liu, S. Fan, S4 : A free electromagnetic solver for layered periodic structures, Computer Physics Communications 183 (10) (2012) 2233–2244. doi:http://dx.doi.org/10.1016/j.cpc.2012.04.026. URL http://www.sciencedirect.com/science/article/pii/S0010465512001658
[51] J. M. Melenk, On generalized finite element methods, PhD Thesis, Univ. of Maryland (1995).

[52] A. Moiola, Trefftz-discontinuous galerkin methods for time-harmonic wave problems, Ph.D. thesis, ETH Zurich (2011).

[53] J. Melenk, Operator adapted spectral element methods I: harmonic and generalized harmonic polynomials, Numer. Math. 84 (1999) 35–69.

[54] J. von Neumann, H. Goldstine, Numerical inverting of matrices of high order, Bull. Amer. Math. Soc. 53 (11) (1947) 1021–1099.

[55] E. P. Wigner, Characteristic vectors of bordered matrices with infinite dimensions, Annals of Mathematics 62 (3) (1955) 548–564. doi:10.2307/1970079.
URL http://www.jstor.org/stable/1970079

[56] G. Akemann, J. Baik, P. D. Francesco, The Oxford Handbook of Random Matrix Theory, Oxford: Oxford University Press, 2011.

[57] T. Tao, V. Vu, Random matrices: the distribution of the smallest singular values, Geometric and Functional Analysis 20 (1) (2010) 260–297. doi:10.1007/s00039-010-0057-8.
URL https://doi.org/10.1007/s00039-010-0057-8

[58] M. Rudelson, R. Vershynin, The least singular value of a random rectangular matrix, Comptes rendus de l’Acadmie des sciences – Mathmatique 346 (2008) 893–896.

[59] M. Rudelson, R. Vershynin, Smallest singular value of a random rectangular matrix, Communications on Pure and Applied Mathematics 62 (12) (2009) 1707–1739. doi:10.1002/cpa.20294.
URL http://dx.doi.org/10.1002/cpa.20294

[60] M. Rudelson, R. Vershynin, Non-asymptotic theory of random matrices: extreme singular values, in: Proceedings of the International Congress of Mathematicians, Hyderabad, India, 2010.