Three types of quasi-Trefftz functions for the 3D convected Helmholtz equation: construction and theoretical approximation properties

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Abstract

Trefftz methods are numerical methods for the approximation of solutions to boundary and/or initial value problems. They are Galerkin methods with particular test and trial functions, which solve locally the governing partial differential equation (PDE). This property is called the Trefftz property. Quasi-Trefftz methods were introduced to leverage the advantages of Trefftz methods for problems governed by variable coefficient PDEs, by relaxing the Trefftz property into a so-called quasi-Trefftz property: test and trial functions are not exact solutions but rather local approximate solutions to the governing PDE. In order to develop quasi-Trefftz methods for aero-acoustics problems governed by the convected Helmholtz equation, the present work tackles the question of the definition, construction and approximation properties of three families of quasi-Trefftz functions: two based on generalizations on plane wave solutions, and one polynomial.

1 Introduction

Several time-harmonic wave propagation phenomena can be modeled by variations of the Helmholtz equation. We are interested in developing tools for the numerical simulation of linear acoustic propagation at a fixed frequency in a subsonic flow in three dimensions. Such phenomena can be modeled by the convected Helmholtz equation for the acoustic potential:

$$- \nabla \cdot (\rho(\nabla \phi - (M \cdot \nabla \phi)M + i\kappa \phi M)) - \rho(\kappa^2 \phi + i\kappa M \cdot \nabla \phi) = 0,$$

(1)

where $\rho$ is the real-valued fluid density and $M$ is the vector-valued fluid velocity, both assumed to be depending on the space variable, while $\kappa$ is the wavenumber. The density $\rho$ is naturally assumed to be positive. We are interested in the subsonic regime, so the Mach number $|M|$ is assumed to be no more than 1. For comparison the standard Helmholtz equation then corresponds to the case of a fluid with velocity equal to zero and a constant density. The methods of interest here are the so-called quasi-Trefftz methods that were introduced as an extension of Trefftz methods for problems of wave propagation in inhomogeneous media.

In a search for bounds on the solutions to boundary value problems, Trefftz introduced in the 1920s the idea to leverage trial functions satisfying the governing equation [33, 29]. Since then, this idea has lead to the development of several numerical methods, generally referred to as Trefftz methods. In the present work, Trefftz methods refer to a class of numerical methods falling within the category of Galerkin methods, and specifically relying on functions that satisfy the governing equation, both for the derivation of their weak formulation and for the discretization of this formulation. Implementing Trefftz methods requires bases of exact solutions to the governing equation - called Trefftz functions - in order to discretize the weak formulation. This then limits their application since exact solutions are not known for many equations. Nevertheless these methods are particularly popular in the field of wave propagation, as circular, spherical, plane or even evanescent waves are some natural and common candidates Trefftz functions, see for instance [30, 26, 13] and references therein. Early works on such methods include the introduction [8, 5] and study [14, 4, 9, 15, 16, 17] of the ultra-weak variational formulation, as well as more general wave-based methods [10, 11, 12]. More recent works include [28, 27] focusing on Trefftz Virtual Element Methods, and [11, 6] focusing on conditioning aspects. Existing extensions to space-time problems include work on acoustics and elasto-acoustics [31, 2], as well as Friedrichs systems [32, 3].

Intuitively, the advantage of Trefftz methods relies on their PDE-dependent function spaces: since Trefftz functions solve exactly the PDE, they can be expected to have better approximation properties than non-PDE dependent function spaces. In practice, local approximation properties of the discrete spaces are a corner stone of convergence properties of Galerkin methods. Typically these would be stated for a space $\mathcal{V}$ of functions to be approximated by functions in a discrete space $\mathcal{V}_h$ locally on some region $\Omega$ as:

$$\forall u \in \mathcal{V}, \exists u_n \in \mathcal{V}_h \text{ s. t. } \forall x \in \Omega, |u(x) - u_n(x)| \leq C|x - x_C|^n.$$
for some order of approximation \( n \). This is precisely where the advantage of Trefftz functions over standard polynomial spaces can be emphasized, as spaces of Trefftz functions require less degrees of freedom to achieve a given order of accuracy than standard polynomial spaces. It is however important to keep in mind that these approximation properties of spaces of Trefftz functions hold only for the approximation of exact solutions to the governing PDE (as will be illustrated in Theorem 2), whereas approximation properties of standard polynomial spaces hold for the approximation of smooth enough function that do not necessarily solve the governing PDE. Bases of Trefftz functions are also known to suffer from ill-conditioning issues in certain regimes, these aspects are beyond the scope of this work.

In the general context of wave propagation, the application of Trefftz methods in their standard form to problems of propagation through inhomogeneous media is similarly limited since one more time global exact solutions are not known for most variable-coefficient equations. Quasi-Trefftz methods, relying on approximate solutions - called quasi-Trefftz functions - rather than exact solutions to the governing equation, were introduced to extend Trefftz methods to problems governed by variable-coefficient equations. They were first introduced in [21] under the name of Generalized Plane Wave (GPW) methods for 2D problems governed by the Helmholtz equation. The original idea behind the GPW concept was to retain the oscillating behavior of a plane wave (PW) while allowing for some extra degrees of freedom to be adapted to the varying PDE coefficient, and this is where their name came from. Initially this was performed via the introduction of Higher Order Terms (HOT) in the phase of a PW as follows:

\[
\left\{ \begin{array}{l}
\varphi(x) = \exp(i\tilde{\kappa}k \cdot x + \text{HOT}) \\
[-\Delta - \kappa^2 \epsilon(x)] \varphi(x) \approx 0,
\end{array} \right.
\]

instead of

\[
\left\{ \begin{array}{l}
\phi(x) = \exp(ik \cdot x) \\
[-\Delta - \kappa^2] \phi = 0,
\end{array} \right.
\]

for any unit vector \( k \in \mathbb{R}^3 \),

(2)

where \( \kappa \) is the wavenumber of the PW while \( \tilde{\kappa} \) can be interpreted as the local wavenumber of the GPW. A procedure to construct a basis of such GPWs was proposed in [18], together with a study of the approximation properties of the basis. A systematic procedure to study these approximation properties was introduced in [24], and used in [19] on a new type of GPWs. The idea of the associated GPW-based Galerkin method was presented in [21], a proof of convergent for a variant was studied in [23]. The method was applied a problem of mode conversion for wave propagation in plasmas in [20].

Other works on quasi-Trefftz methods include [34] on the convergence of a GPW Discontinuous Galerkin method for anisotropic Helmholtz problems, [3], on linear transport problems, as well as [22] on time-dependent wave propagation problems.

Quasi-Trefftz methods rely on function spaces of approximate solutions to the governing equation, as opposed to exact solutions, and this is their fundamental property. In our work, we define this approximation as a local property in the sense of a Taylor expansion. Given the partial differential operator \( L \) of the governing equation, and any point \( x_C \) in the domain of interest, we consider functions \( \varphi \) with the following property:

\[
L \varphi(x) = O(|x - x_C|^q),
\]

for some parameter \( q \) providing some flexibility in the desired order of approximation with respect to the distance \( |x - x_C| \). In other words the degree \( q - 1 \) Taylor polynomial of the image of \( \varphi \) through the operator \( L \) is zero. In the context of Discontinuous Galerkin methods, with function spaces of local functions defined element-wise on a computational mesh, then if (3) holds within each element, with \( x_C \) in the element, then the remainder can be described as \( O(h^q) \) where \( h \) denotes the mesh size, as \( |x - x_C| \leq h \) for all \( x \) in the element. There the goal is to establish so-called \( h \)-convergence properties, that is in the regime \( h \rightarrow 0 \). Note that, in order to prove their convergence, quasi-Trefftz methods so far include in their weak formulations a stabilization term to handle the non-zero remainder in the quasi-Trefftz property (3), see [23] [34] [22].

1.1 Central results

Our goal is to address here the fundamental question of basis functions at the centre of quasi-Trefftz methods for the three-dimensional convected Helmholtz equation: the actual construction of basis functions is fundamental to the discretization stage, and therefore to the implementation of the methods, while the
approximation properties of the discrete space are a fundamental element in the proof of convergence of the methods. Since quasi-Trefftz functions satisfy a local quasi-Trefftz property \(3\), more precisely, the goal of this work is twofold:

1. developing algorithms for the construction of local basis functions for quasi-Trefftz function spaces for the partial differential operator of the three-dimensional convected Helmholtz equation, \(\nabla h\), guaranteeing a limited computational cost for the practical construction,

2. studying the local approximation property of the resulting spaces \(\mathbb{V}_h\) in the following sense; given \(n \in \mathbb{N}\), there is a space \(\mathbb{V}_h\) satisfying:

\[
\forall u \text{ satisfying the governing PDE, } \exists u_a \in \mathbb{V}_h \text{ s.t. } \forall x \in \mathbb{R}^3, |u(x) - u_a(x)| \leq C|x - x_C|^{n+1}. \quad (4)
\]

Inspired by classical PWs \(\exp \Lambda \cdot (x - x_C)\), we will focus on three different families of quasi-Trefftz functions:

- phase-based GPWs, following the original ansatz proposed in \(21\) via the introduction of higher order terms in the phase of a PW, see \(2\).
- amplitude-based GPWs, following the ansatz proposed in \(19\) via the introduction of higher order terms in the amplitude of a PW,
- purely polynomial quasi-Trefftz functions, which so far we have only used for time-dependent wave propagation in \(22\).

In each of the wave-based cases the ansatz is an extension of cases studied previously in two-dimensions, whereas the situation is different for the polynomial case. This is the first time that polynomial quasi-Trefftz functions are proposed for time-harmonic problems.

We will pursue the announced goals for these three families of quasi-Trefftz functions, highlighting the similarities and differences between the three cases. The fundamental contribution of this work is to show that these three families of quasi-Trefftz functions achieve the approximation properties with exactly the same number of degrees of freedom as their Trefftz function (wave-based) counterpart do for the constant-coefficient cases studied in the literature.

It is important to note that general time-harmonic wave-propagation equations have no exact polynomial solution, in other words there exist no polynomial Trefftz function in this case. However, there are more quasi-Trefftz functions than Trefftz functions, since the former are defined by a less restrictive constraint, and as we will see there exist polynomial quasi-Trefftz functions.

1.2 Preliminaries

Throughout this article, we will use the following notation. The canonical basis of \(\mathbb{R}^3\) or \((\mathbb{N}_0)^3\) is denoted \(\{e_k, k \in \{1, 2, 3\}\}\), and \(| \cdot |\) denotes the euclidean norm on \(\mathbb{R}^3\). The set of positive integers is denoted \(\mathbb{N}\) and the set of non-negative integers is denoted \(\mathbb{N}_0 := \mathbb{N} \cup \{0\}\), while the zero multi-index is denoted \(0 = (0, 0, 0)\).

Multi-indices in \((\mathbb{N}_0)^3\) are denoted \(\alpha, \beta, i, j\), the sum of multi-indices is defined as \(i + j = (i_1 + j_1, i_2 + j_2, i_3 + j_3)\) for all \(i\) and \(j\) in \((\mathbb{N}_0)^3\) while \(| \cdot |\) also denotes the length for a multi-index, that is \(|i| = i_1 + i_2 + i_3\) for all \(i \in (\mathbb{N}_0)^3\), and for the sake of compactness \(i \leq j\) means that \(i_k \leq j_k\) for \(k \in \{1, 2, 3\}\), \(i < j\) means that \(i \neq j\) and \(i_k \leq j_k\) for \(k \in \{1, 2, 3\}\), and the linear order \(<\) on \(\mathbb{N}_0^3\) is defined by

\[
\forall (\mu, \nu) \in (\mathbb{N}_0^3)^2, \mu < \nu \Leftrightarrow \left\{ \begin{array}{ll} |\mu| < |\nu|, & \text{or} \\ |\mu| = |\nu| \text{ and } \mu_1 < \nu_1, & \text{or} \\ |\mu| = |\nu|, \mu_1 = \nu_1 \text{ and } \mu_2 < \nu_2. \end{array} \right.
\]

The generic point of interest in the domain of the equation is denoted \(x_C\). The coefficient of a Taylor expansion in the neighborhood of \(x_C\), for any \(n \in \mathbb{N}\), are denoted \(T_f[\beta] = \frac{1}{\beta!} \partial_x^\beta f(x_C)\) for all function \(f \in \mathbb{C}^n\) at \(x_C\) with \(\beta \in \mathbb{N}_0^3, |\beta| \leq n\). We chose to avoid an unnecessary explicit mention of \(x_C\) in the \(T\) notation because all Taylor expansion will be performed at \(x_C\).
Remark 1. Given \( n \in \mathbb{N}_0 \) and \( x_C \in \mathbb{R}^3 \), a few simple derivative rules can then be expressed in a compact way as follows:

\[
\begin{align*}
T_f g[\beta] &= \sum_{\gamma \leq \beta} T_f[\beta - \gamma] T_g[\gamma] \quad \text{if } f \text{ and } g \text{ are } \mathcal{C}^n \text{ at } x_C \text{ with } |\beta| \leq n, \\
T_{fgh}[\beta] &= \sum_{\gamma \leq \beta} \sum_{\eta \leq \gamma} T_f[\beta - \gamma] T_g[\gamma - \eta] T_h[\eta - \eta], \\
T_{\partial^2_f}[\beta] &= \frac{(\alpha + \beta)!}{\beta!} T_f[\alpha + \beta] \quad \text{if } f \text{ is } \mathcal{C}^n \text{ at } x_C \text{ with } |\alpha| + |\beta| \leq n, \\
T_{(X-x_C)^i}[\beta] &= \delta(\beta - i).
\end{align*}
\]

Definition 1. A linear partial differential operator of order 2, in three dimensions, with a given set of complex-valued functions \( c = \{c_i; i \in \mathbb{N}_0^3, |i| \leq 2\} \) will be denoted hereafter as

\[
\mathcal{L}_c := \sum_{i \in \mathbb{N}_0^3, |i| \leq 2} c_i(x) \partial_x^i,
\]

where \( x = (x_1, x_2, x_3) \in \mathbb{R}^3 \) and \( \partial_x^i = \partial_{x_1}^{i_1} \partial_{x_2}^{i_2} \partial_{x_3}^{i_3} \).

We will make use of the fact that the set \( \{ i \in \mathbb{N}_0^3, |i| \leq 2 \} \) can be split as:

\[
\{ i \in \mathbb{N}_0^3, |i| \leq 2 \} = \{ 2e_k, 1 \leq k \leq 3 \} \cup \{ e_k + e_{k'}, 1 \leq k < k' \leq 3 \} \cup \{ e_k, 1 \leq k \leq 3 \} \cup \{ 0 \}
\]

For instance, in the case of the convected Helmholtz equation, the variable coefficients of the partial differential operator can then be defined as follows:

\[
\begin{align*}
c_{2e_k} &= \rho (M_k)^2 - 1 \quad \text{for } 1 \leq k \leq 3, \\
c_{e_k + e_l} &= \rho M_k M_l \quad \text{for } 1 \leq k < k' \leq 3, \\
c_{e_k} &= \rho \sum_{i} M_i \partial_{x_i} M_k + \nabla \cdot (\rho M) M_k - \partial_{x_k} \rho - 2i\kappa \rho M_k \quad \text{for } 1 \leq k \leq 3, \\
c_0 &= -i\kappa^2 \nabla \cdot (\rho M) - \rho \kappa^2.
\end{align*}
\]

Beyond the convected Helmholtz equation, the work proposed in this article relies on a set of minimal hypotheses for the partial differential operator \( \mathcal{L}_c \). The first aspect will lead to the well-posedness of a subproblem in the construction of quasi-Trefftz functions, whereas the second will lead to the construction of a set of linearly independent quasi-Trefftz functions. We gather the two in the following Hypothesis.

Hypothesis 1. Given a point \( x_C \in \mathbb{R}^3 \) and a set of complex-valued functions \( c = \{c_i; i \in \mathbb{N}_0^3, |i| \leq 2\} \), the functions are assumed to be \( \mathcal{C}^\infty \) at the point \( x_C \), with \( c_{2e_1}(x_C) \neq 0 \) and the matrix defined by:

\[
\mathcal{C} := \begin{bmatrix}
T_{c_{2e_1}}[0] & \frac{1}{2} T_{c_{e_1+e_2}}[0] & \frac{1}{2} T_{c_{e_1+e_3}}[0] \\
\frac{1}{2} T_{c_{e_1+e_2}}[0] & T_{c_{2e_2}}[0] & \frac{1}{2} T_{c_{e_2+e_3}}[0] \\
\frac{1}{2} T_{c_{e_1+e_3}}[0] & \frac{1}{2} T_{c_{e_2+e_3}}[0] & T_{c_{2e_3}}[0]
\end{bmatrix}
\]

is non-singular. As a consequence, there are two real matrices, an orthogonal matrix \( \mathcal{P} \) and a non-singular diagonal matrix \( \mathcal{D} \), depending only on the set of coefficients \( c \) evaluated at \( x_C \), such that \( \mathcal{C} = \mathcal{P} \mathcal{D} \mathcal{P}^T \).

The convected Helmholtz operator satisfies Hypothesis 1 according to the following comments.

- The density \( \rho(x_C) \) is positive, and there is at least one index \( k \in \{1, 2, 3\} \) such that \( M_k(x_C) \neq 1 \) since the Mach number is assumed to be no more than 1, \( |M(x_C)| < 1 \). Hence \( \rho(x_C)((M_k)^2(x_C) - 1) \neq 0 \), in other words in particular we indeed have \( c_{2e_1} \neq 0 \).
• The matrix $\mathcal{C}$ defined by:

$$
\begin{bmatrix}
T_{c_{e_1}}[0] & \frac{1}{2}T_{c_{e_1}+\epsilon_2}[0] & \frac{1}{2}T_{c_{e_1}+\epsilon_3}[0] \\
\frac{1}{2}T_{c_{e_1}+\epsilon_2} & T_{c_{e_2}}[0] & \frac{1}{2}T_{c_{e_2}+\epsilon_3}[0] \\
\frac{1}{2}T_{c_{e_1}+\epsilon_3} & \frac{1}{2}T_{c_{e_2}+\epsilon_3} & T_{c_{e_3}}[0]
\end{bmatrix}
\
= \rho(x_C) \begin{bmatrix}
(M_1(x_C))^2 - 1 & \frac{1}{2}M_1(x_C)M_2(x_C) & \frac{1}{2}M_1(x_C)M_3(x_C) \\
\frac{1}{2}M_1(x_C)M_2(x_C) & \left(M_2(x_C)\right)^2 - 1 & \frac{1}{2}M_2(x_C)M_3(x_C) \\
\frac{1}{2}M_1(x_C)M_3(x_C) & \frac{1}{2}M_2(x_C)M_3(x_C) & \left(M_3(x_C)\right)^2 - 1
\end{bmatrix},
$$

is related to the second order terms in the partial differential operator, and the density $\rho(x_C)$ is positive. Under the assumption that $|M(x_C)| < 1$ it can be shown that $1/\rho(x_C)\mathcal{C}$ is non-singular, see appendix A. Hence since the Mach number is assumed to be no greater than 1, the matrix $\mathcal{C}$ is indeed non-singular.

Finally, $\{\lambda_i, \mu_i, \nu_i, i \in (\mathbb{N}_0)^3\}$ denote complex polynomial coefficients, and, for a given integer $d$, we denote the corresponding polynomials:

$$
P := \sum_{i \in \mathbb{N}_0^3, |i| \leq d} \lambda_i X^i, \quad Q := \sum_{i \in \mathbb{N}_0^3, |i| \leq d} \mu_i X^i \text{ and } R := \sum_{i \in \mathbb{N}_0^3, |i| \leq d} \nu_i X^i, \text{ where } X^i = X_1^{i_1} X_2^{i_2} X_3^{i_3}.
$$

As a convention, when referring to a polynomial of degree at most equal to $d$ we include the zero polynomial.

## 2 Three types of quasi-Trefftz functions

The quasi-Trefftz property for a function is a property of the image of this function under the action of the partial differential operator. Two fundamental aspects of this property are related to its statement in terms of a Taylor expansion approximation: (i) the fact that it is a local property, and (ii) the fact that it allows for a choice in the desired order of approximation. Hence, as it relies on enforcing the quasi-Trefftz property, the construction of quasi-Trefftz functions is performed at a given point $x_C$ and constructed functions satisfy the property at a given order of approximation $q$.

The first question is obviously that of the existence of quasi-Trefftz functions. A second question is nevertheless equally important for the efficient implementation of quasi-Trefftz methods, that of the computational cost of the practical construction of quasi-Trefftz bases. Indeed, the construct the quasi-Trefftz functions is only a pre-computation to the discretization of a quasi-Trefftz weak formulation, therefore its computational cost must be acceptable compared to that of the assembly of the discrete matrix and the resolution of the linear system. The former question will be addressed by the derivation of an algorithm for the construction of quasi-Trefftz functions. The latter question will be settled by the precise steps of the construction algorithm, as the algorithm only applies explicit closed formulas while it requires no numerical resolution of any system.

In this section, we present three types of quasi-Trefftz functions.

• The original GPW ansatz, namely exp $\left(\Lambda \cdot (x - x_C) + \text{HOT}\right)$, introduced higher order terms in the phase of a PW. The general form of this ansatz can be described as exp $P(x - x_C)$, for some polynomial $P$.

• In comparison, a new ansatz was proposed via the introduction of higher order terms in the amplitude of a PW as $(1 + \text{HOT}) \exp \Lambda \cdot (x - x_C)$. Therefore such an ansatz has the general form $Q(x - x_C) \exp \Lambda \cdot (x - x_C)$, for some polynomial $Q$ and some $\Lambda$.

• Moreover, we propose here to consider purely polynomial quasi-Trefftz functions, described as $R(x - x_C)$ for some polynomial $R$. 

To guarantee the existence of such quasi-Trefftz function, we will study the existence of polynomials \((P, Q \text{ or } R)\) such that the associated ansatz satisfies the desired quasi-Trefftz property \(\text{(3)}\). To do so we will conveniently reformulate the problem to evidence properties of the resulting system, underlining the shared common structure of these systems. These properties will appear to be central to the construction of quasi-Trefftz functions.

### 2.1 Amplitude-based GPWs

Initially, the abstract problem of construction of an amplitude-based GPW can be written, for a given \(q \in \mathbb{N}\), as:

\[
\begin{align*}
\text{Find } (Q, \Lambda) &\in \mathbb{C}[X_1, X_2, X_3] \times \mathbb{C}^3 \text{ such that} \\
J(x) &:= Q(x - x_C) \exp \Lambda \cdot (x - x_C) \text{ satisfies} \\
\mathcal{L}_c J(x) &= O(|x - x_C|^q)
\end{align*}
\]

The unknowns here are of two types, either polynomial, for \(Q\), or scalar, for the three components of \(\Lambda\), and the specific role of \(\Lambda\) will be highlighted throughout the discussion. To formulate a more concrete problem, we focus on the action of the differential operator \(\mathcal{L}_c\) on the ansatz. If \(J(x) := Q(x - x_C) \exp \Lambda \cdot (x - x_C)\) with \(Q \in \mathbb{C}[X_1, X_2, X_3]\) and \(\Lambda \in \mathbb{C}^3\), then

\[
\mathcal{L}_c J(x) = \left( \sum_{k=1}^{3} c_{2e_k}(x) \left( \partial_x^{2e_k} Q(x - x_C) + 2\Lambda_k \partial_x^{e_k} Q(x - x_C) + \Lambda_k^2 Q(x - x_C) \right) \right)
\]

\[
+ \sum_{1 \leq k < k' \leq 3} c_{e_k + e_k'}(x) \left( \partial_x^{e_k + e_k'} Q(x - x_C) + \Lambda_k \partial_x^{e_k} Q(x - x_C) + \Lambda_k \partial_x^{e_k'} Q(x - x_C) + \Lambda_k \Lambda_k' Q(x - x_C) \right)
\]

\[
+ \sum_{k=1}^{3} c_{e_k}(x) \left( \partial_x^{e_k} Q(x - x_C) + \Lambda_k Q(x - x_C) \right) + c_0(x) Q(x - x_C) \right) \exp \Lambda \cdot (x - x_C).
\]

We can then define the partial differential operator

\[
\mathcal{L}_c^{\text{Am.}\Lambda} Q(x) := \left( \sum_{k=1}^{3} c_{2e_k}(x) \left( \partial_x^{2e_k} Q(x - x_C) + 2\Lambda_k \partial_x^{e_k} Q(x - x_C) + \Lambda_k^2 Q(x - x_C) \right) \right)
\]

\[
+ \sum_{1 \leq k < k' \leq 3} c_{e_k + e_k'}(x) \left( \partial_x^{e_k + e_k'} Q(x - x_C) + \Lambda_k \partial_x^{e_k} Q(x - x_C) + \Lambda_k \partial_x^{e_k'} Q(x - x_C) + \Lambda_k \Lambda_k' Q(x - x_C) \right)
\]

\[
+ \sum_{k=1}^{3} c_{e_k}(x) \left( \partial_x^{e_k} Q(x - x_C) + \Lambda_k Q(x - x_C) \right) + c_0(x) Q(x - x_C)
\]

to emphasize that

\[
\mathcal{L}_c J(x) = \left( \mathcal{L}_c^{\text{Am.}\Lambda} Q(x) \right) \exp \Lambda \cdot (x - x_C),
\]

where for \(\Lambda \in \mathbb{C}^3\) the exponential term is locally bounded. As a result, for \(J\) to satisfy the desired property \(\mathcal{L}_c J(x) = O(|x - x_C|^q)\), it is then sufficient for \(\Lambda\) and \(Q\) to satisfy \(\mathcal{L}_c^{\text{Am.}\Lambda} Q(x) = O(|x - x_C|^q)\). Therefore we will formulate a new problem for construction of GPWs

\[
\begin{align*}
\text{Find } (Q, \Lambda) &\in \mathbb{C}[X_1, X_2, X_3] \times \mathbb{C}^3 \text{ such that} \\
\mathcal{L}_c^{\text{Am.}\Lambda} Q(x) &= O(|x - x_C|^q) \\
\text{then } J(x) &:= Q(x - x_C) \exp \Lambda \cdot (x - x_C)
\end{align*}
\]

and any solution \(J\) to \((6)\) will be solution to the initial problem \((5)\).

We can now express a concrete problem in terms of scalar equations and scalar unknowns thanks to Remark \(\text{1}\) the equations corresponding to cancelling the Taylor expansion coefficients of \(\mathcal{L}_c^{\text{Am.}\Lambda} Q\) for orders
from 0 to \(q - 1\) and the unknowns corresponding to all the free parameters defining the GPW namely the \(\mu\)s and \(\Lambda\). Indeed, (6) can equivalently be stated as follows as long as \(d \geq q + 1\):

\[
\begin{align*}
\text{Find } \Lambda \in \mathbb{C}^3 \text{ and } \{\mu_i \in \mathbb{C}, i \in \mathbb{N}_0^3, |i| \leq d\} \text{ satisfying } \forall \beta \text{ such that } |\beta| < q \\
&\quad \sum_{\gamma \leq \beta} \left( \sum_{k=1}^3 T_{c_{e_k}}[\beta - \gamma] \left( (\gamma_k + 1)(\gamma_k + 1)\mu_{\gamma+2e_k} + 2\Lambda_k(\gamma_k + 1)\mu_{\gamma+e_k} + \Lambda_k^2 \mu_{\gamma} \right) \\
&\quad + \sum_{1 \leq k \neq k' \leq 3} T_{c_{e_k+e_{k'}}}[\beta - \gamma] \left( (\gamma_k + 1)(\gamma_{k'} + 1)\mu_{\gamma+e_k+e_{k'}} + \Lambda_k(\gamma_{k'} + 1)\mu_{\gamma+e_{k'}} + \Lambda_{k'}(\gamma_k + 1)\mu_{\gamma+e_k} + \Lambda_k\Lambda_{k'}\mu_{\gamma} \right) \\
&\quad + \sum_{k=1}^3 T_{c_{e_k}}[\beta - \gamma] \left( (\gamma_k + 1)\mu_{\gamma+e_k} + \Lambda_k \mu_{\gamma} \right) + T_{c_0}[\beta - \gamma] \mu_{\gamma} \right) = 0, \\
\end{align*}
\]

(7)

if \(\{\mu_i\}\) is the set of polynomial coefficients of \(Q\). The choice \(d \geq q + 1\) simply ensures that all equations have the same structure. Indeed, for instance, there would be no \(\mu_{\beta+2e_k}\) term in \(T_{\mathcal{L}_c^{\beta m}\Lambda Q}[\beta]\) for \(|\beta| = q\) if we chose \(d < q + 1\). Hence we will always consider the case:

\[
d \geq q + 1
\]

2.2 Phase-based GPWs

Similarly, the abstract problem of construction of a phase-based GPW can initially be written, for a given \(q \in \mathbb{N}\), as:

\[
\begin{align*}
\text{Find a polynomial } P \in \mathbb{C}[X_1, X_2, X_3] \text{ such that } \\
G(x) := \exp P(x - x_C) \text{ satisfies } \\
\mathcal{L}_c G(x) = O(|x - x_C|^q). \\
\end{align*}
\]

(8)

Thanks to the definition of the partial differential operator

\[
\mathcal{L}_c^P\!^h P(x) := \sum_{k=1}^3 c_{2e_k}(x) \left( \partial_x^{2e_k} P(x - x_C) + (\partial_x^{e_k} P(x - x_C))^2 \right) \\
+ \sum_{1 \leq k \neq k' \leq 3} c_{e_k+e_{k'}}(x) \left( \partial_x^{e_k+e_{k'}} P(x - x_C) + \partial_x^{e_k} P(x - x_C) \partial_x^{e_{k'}} P(x - x_C) \right) \\
+ \sum_{k=1}^3 c_{e_k}(x) \partial_x^{e_k} P(x - x_C) + c_0(x),
\]

we can easily verify that

\[
\mathcal{L}_c G(x) = \left( \mathcal{L}_c^P\!^h P(x) \right) \exp P(x - x_C).
\]

Hence any solution \(G\) to the problem:

\[
\begin{align*}
\text{Find a polynomial } P \in \mathbb{C}[X_1, X_2, X_3] \text{ such that } \\
\mathcal{L}_c^P\!^h P(x) = O(|x - x_C|^q) \\
\text{ then } G(x) := \exp P(x - x_C) \\
\end{align*}
\]

(9)
will also be a solution to the initial problem \( \mathfrak{S} \). In terms of scalar unknowns and equations, as long as \( d \geq q + 1 \), this is then equivalent to:

\[
\begin{align*}
\text{Find } \{ \lambda_i \in \mathbb{C}, i \in \mathbb{N}_0^d, |i| \leq d \} \text{ satisfying } \forall \beta & \text{ such that } |\beta| < q \\
\sum_{\gamma \leq \beta} \left( \sum_{k=1}^3 T_{c\omega k}[\beta - \gamma] \left( (\gamma_k + 2)(\gamma_k + 1)\lambda_{\gamma_2 e_k} + \sum_{\eta \leq \gamma} (\gamma_k - \eta_k + 1)\lambda_{\gamma - \eta + \epsilon_k} (\eta_k + 1)\lambda_{\eta + e_k} \right) \\
+ \sum_{1 \leq k < k' \leq 3} T_{c\omega k + e_k}[\beta - \gamma] \left( (\gamma_k + 1)(\gamma_{k'} + 1)\lambda_{\gamma + e_k + e_{k'}} + \sum_{\eta \leq \gamma} (\gamma_{k'} - \eta_{k'} + 1)\lambda_{\gamma - \eta + e_{k'}} (\eta_k + 1)\lambda_{\eta + e_k} \right) \\
+ \sum_{k=1}^3 T_{c\omega k}[\beta - \gamma](\gamma_k + 1)\lambda_{\gamma + e_k} + T_{c\alpha}[\beta - \gamma]\nu_{\gamma} \right) = 0,
\end{align*}
\]

(10)

if \( \{ \lambda_i \} \) is the set of polynomial coefficients of \( P \). Similarly here the choice \( d \geq q + 1 \) simply ensures that all equations have the same structure.

### 2.3 Polynomial functions

The abstract problem of construction of a purely polynomial quasi-Trefftz function can simply be written, for a given \( q \in \mathbb{N} \), as:

\[
\begin{align*}
\text{Find a polynomial } R \in \mathbb{C}[X_1, X_2, X_3] \text{ such that } \\
H(x) := R(x - x_C) \text{ satisfies } \\
\mathcal{L}_c H(x) = O(|x - x_C|^q).
\end{align*}
\]

(11)

In terms of scalar unknowns and equations, as long as \( d \geq q + 1 \) to ensure again that all equations have the same structure, this is equivalent to:

\[
\begin{align*}
\text{Find } \{ \nu_i \in \mathbb{C}, i \in \mathbb{N}_0^d, |i| \leq d \} \text{ satisfying } \forall \beta & \text{ such that } |\beta| < q \\
\sum_{\gamma \leq \beta} \left( \sum_{k=1}^3 T_{c\omega k}[\beta - \gamma](\gamma_k + 2)(\gamma_k + 1)\nu_{\gamma_2 e_k} \\
+ \sum_{1 \leq k < k' \leq 3} T_{c\omega k + e_k}[\beta - \gamma](\gamma_k + 1)(\gamma_{k'} + 1)\nu_{\gamma + e_k + e_{k'}} \\
+ \sum_{k=1}^3 T_{c\omega k}[\beta - \gamma](\gamma_k + 1)\nu_{\gamma + e_k} + T_{c\alpha}[\beta - \gamma]\nu_{\gamma} \right) = 0,
\end{align*}
\]

(12)

if \( \{ \nu_i \} \) is the set of polynomial coefficients of \( R \).

### 2.4 Common structure

These systems share common aspects but also exhibit differences. We will leverage the former to derive very similar construction algorithms for the three types of quasi-Trefftz functions.

The unknowns in both systems (7), (10) and (12) include the \((d+1)(d+2)(d+3)/6\) polynomial coefficients, respectively \( \{ \mu_i \in \mathbb{C}, i \in \mathbb{N}_0^d, |i| \leq d \}, \{ \lambda_i \in \mathbb{C}, i \in \mathbb{N}_0^d, |i| \leq d \}, \) and \( \{ \nu_i \in \mathbb{C}, i \in \mathbb{N}_0^d, |i| \leq d \}, \) while only in the amplitude-based case there are three additional scalar unknowns, \( \Lambda \in \mathbb{C}^3 \). In the polynomial case the system is linear, whereas in both GPW cases the systems are non-linear. However in the amplitude-based case the non-linear terms are limited to products of one \( \mu_i \) and powers of \( \Lambda \).

Besides, each system has \( q(q + 1)(q + 2)/6 \) equations, and we will now describe their common layer structure. A close inspection of the equations reveals an underlying structure linked to the unknowns’ and equations’ multi-indices. Indeed, for any equation \( \beta \), unknowns \( \mu_i \) or \( \lambda_i \) with \( |i| \leq |\beta| + 1 \) may appear in non-linear terms, whereas unknowns \( \mu_i, \lambda_i \) or \( \nu_i \) with \( |i| = |\beta| + 2 \) can only appear in linear terms. This is summarized in the following two tables.
We have seen that in each case choosing $d \geq q + 1$ ensures that all equations of the system share a common structure. It is straightforward to see from these tables that none of the $\mu$, $\lambda$ or $\nu$ unknowns with indices $i \in \mathbb{N}^3$ such that $|i| > q + 1$ appear in the system since $|\beta| \leq q - 1$. Hence these unknowns are not constrained by the system: their values do not affect the system - and therefore neither do they affect the quasi-Trefftz property - even though they would of course affect the definition of the corresponding quasi-Trefftz function. As a result, it is sufficient to seek a polynomial $P$, $Q$ and $R$ of degree $d$ satisfying:

$$d = q + 1$$

As we can see from the Comments columns of the previous tables, all non-linear terms involve unknowns with multi-indices of length at most equal to $|\beta| + 1$, while the only unknowns with multi-indices of length $|\beta| + 2$ are $\mu_{\beta+e_k}$, $\lambda_{\beta+e_k}$ or $\nu_{\beta+e_k}$ with $1 \leq k \leq k' \leq 3$. The length of multi-indices then plays an important role in the structure of the system. Hence, in the index space $(\mathbb{N}_0)^3$, we describe the set of multi-indices of a given length $\ell$ as a layer, as illustrated in Figure 1. In order to take advantage of the systems layer structure, we will now split the sets of equations and unknowns according to their multi-index lengths.

Let’s consider, for $\ell \in \mathbb{N}_0$ with $\ell < q$, the subset of equations corresponding to $|\beta| = \ell$. From our previous observations we know that all the terms involving unknowns with multi-index length equal to $\ell + 2$, namely $\mu_{\beta+e_k}$, $\lambda_{\beta+e_k}$ or $\nu_{\beta+e_k}$ with $1 \leq k \leq k' \leq 3$, are linear. Hence if unknowns with a shorter multi-index - and the $\Lambda$ unknowns in the amplitude-based case – were already known, it would suggest, for $\ell \in \mathbb{N}_0$ with $\ell < q$, to define a linear underdetermined subsystem with:
Figure 1: Illustration of a multi-index layer in \((\mathbb{N}_0)^3\). The layer \(\{n \in \mathbb{N}_0^3, |n| = \ell\}\) for \(\ell = 7\) is represented in blue. All elements in the layer are represented as blue dots, the element \(n = (3, 1, 3)\) is highlighted in white.

- \(\frac{(\ell+1)(\ell+2)}{2}\) equations, namely the equations corresponding to \(\beta\) with \(|\beta| = \ell\),
- \(\frac{(\ell+3)(\ell+4)}{2}\) unknowns, namely the unknowns \(\{\mu_i, |i| = \ell + 2\}, \{\lambda_i, |i| = \ell + 2\}\) or \(\{\nu_i, |i| = \ell + 2\}\),
- a right hand side depending on \(\{\mu_i, |i| < \ell + 2\} \cup \Lambda, \{\lambda_i, |i| < \ell + 2\}\), or \(\{\nu_i, |i| < \ell + 2\}\).

To ensure that the right hand side is known at each layer \(\ell\), it is then only natural to proceed layer by layer for increasing values of \(\ell\) from 0 to \(q - 1\).

The construction of a solution to the initial system, \((7), (10)\) or \((12)\), then boils down to the successive construction of a solution to each subsystem. In each case, a set of subsystems gathers \(1/2 \sum_{\ell=0}^{q-1} (\ell+1)(\ell+2) = q(q+1)(q+2)/6\) equations, so that is exactly the full set of equations of the initial system. From the point of view of unknowns the situation is different. Aside from the \(1/2 \sum_{\ell=0}^{q-1} (\ell+3)(\ell+4) = q(q^2 + 9q + 26)/6\) unknowns appearing in the combined subsystems, we immediately notice that the unknowns \(\{\mu_i, |i| \leq 1\}\), \(\Lambda, \{\lambda_i, |i| \leq 1\}\), and \(\{\nu_i, |i| \leq 1\}\) do not belong to any set of subsystem unknowns, but only appear in right hand sides of the subsystems. So the subsystems’ solvability won’t be affected by these terms, yet their values need to be fixed in order for the subsystem’s right hand sides to be known. The construction of a solution to the initial system will hence start from setting the values of \(\{\mu_i, |i| \leq 1\}\) and \(\Lambda, \{\lambda_i, |i| \leq 1\}\), the values of \(\{\nu_i, |i| \leq 1\}\) or the values of \(\{\nu_i, |i| \leq 1\}\) before turning to the hierarchy of subsystems for increasing values of \(\ell\) from 0 to \(q - 1\).

Not only do the amplitude and phase based cases share the same layer structure, but their subsystems also share the same structure. Indeed, independently of the case, for a given layer \(\ell\), the subsystem reads as

\[
\begin{cases}
    \text{Find } \{\xi_i \in \mathbb{C}, i \in \mathbb{N}_0^3, |i| = \ell + 2\} \text{ satisfying } \forall \beta \text{ such that } |\beta| = \ell \\
    \sum_{k=1}^{3} (\beta_k + 2)(\beta_k + 1)T_{c_{2k}}[0]\xi_{\beta+2e_k} \\
    + \sum_{1 \leq k < k' \leq 3} (\beta_k + 1)(\beta_{k'} + 1)T_{c_{k+e_{k'}}}[0]\xi_{\beta+e_k+e_{k'}} = B_{\beta},
\end{cases}
\]
where the right hand side $B$ depends not only on the case but also on variable coefficients of the PDE. As a consequence, the study of existence of solutions to these subsystems is independent of the case. These subsystems will be the backbone of the construction algorithm for both families of GPWs.

**Remark 2.** Gathering unknowns according to the length of their index, $|i|$, is related to splitting the unknowns from the polynomial $P$, $Q$ or $R$ according to the total degree of each monomial:

$$P = \sum_{\ell' = 0}^{q+1} \left( \sum_{|i| = \ell'} \lambda_i X^i \right), \quad Q = \sum_{\ell' = 0}^{q+1} \left( \sum_{|i| = \ell'} \mu_i X^i \right), \quad or \quad R = \sum_{\ell' = 0}^{q+1} \left( \sum_{|i| = \ell'} \nu_i X^i \right),$$

and the $\ell$th subsystem is related to certain derivatives of homogeneous polynomials of degree $\ell' = \ell + 2$.

The subsystems are linear and underdetermined. Their right hand sides depend on the Taylor expansion coefficients of the set of complex-valued PDE coefficients $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$, as well as other unknowns hopefully previously computed. Let’s now turn to the question of existence of solutions to each subsystem.

### 2.5 Subsystems

To proceed, following Remark 2 we will denote by $\mathbb{A} = \mathbb{C}[X]$ the space of complex polynomials in three variables, $X = (X,Y,Z)$, and by $\mathbb{A}_d \subset \mathbb{A}$ the space of homogeneous polynomials of degree $d$. In order to prove the existence of a solution to each linear subsystem, we therefore introduce the partial differential operator

$$\Delta_{c,\ell} : \mathbb{A}_{\ell+2} \rightarrow \mathbb{A}_\ell, \quad f \mapsto \Delta_c f$$

where, given the set of complex-valued PDE coefficients $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$, the linear operator $\Delta_c$ is defined on $\mathbb{A}$ by

$$\begin{cases}
\Delta_c \left[ \sum_{i \in (\mathbb{N}_0^3), |i| < 2} \xi_i X^i \right] = 0, \\
\text{if } d \geq 2, \Delta_c \left[ \sum_{i \in (\mathbb{N}_0^3), |i| \leq d} \xi_i X^i \right] = \sum_{|\beta|-d-2} \left( \sum_{k=1}^{3} (\beta_k + 2)(\beta_k + 1)T_{c_{\beta_k}} [0] \xi_{\beta+2e_k} \right. \\
\left. + \sum_{1 \leq k < k' \leq 3} (\beta_k + 1)(\beta_{k'} + 1)T_{c_{\beta_k+e_k}c_{\beta_{k'}+e_{k'}}} [0] \xi_{\beta+e_k+e_{k'}} \right) X^\beta.
\end{cases}$$

The existence of solutions to (13) is equivalent to the surjectivity of the operator $\Delta_{c,\ell}$. While $\dim \mathbb{A}_{\ell+2} = (\ell + 3)(\ell + 4)/2$ and $\dim \mathbb{A}_\ell = (\ell + 1)(\ell + 2)/2$, unfortunately, it is not simple here to express explicitly the kernel of $\Delta_{c,\ell}$ to find its dimension, unlike for the 2D Laplacian operator. However, we can evidence the operator’s full-rank by exhibiting the echelon structure of a particular matrix representation of $\Delta_{c,\ell}$ in appropriate bases. To describe such a matrix, we will use the canonical bases of $\mathbb{A}_L$ for $L \in \{\ell, \ell+2\}$, namely $\{X^i, i \in \mathbb{N}_0^3, |i| = L\}$, and we will number the columns for $L = \ell + 2$ and the rows for $L = \ell$ according to the linear order $<$ defined for multi-indices $i \in \mathbb{N}_0^3$ with a given length $L$ by

$$\forall (i, j) \in (\mathbb{N}_0^3)^2, i < j \text{ if } \begin{cases}
i_1 < j_1; \text{ or } \\
i_1 = j_1 \text{ and } i_2 < j_2,
\end{cases}$$

while $|i| = L$ and $|j| = L$, so $i_3 = L - i_1 - i_2$ and similarly $j_3 = L - j_1 - j_2$. On each row $\beta$ of the matrix, the only non-zero terms are

| Column index | Matrix entry |
|--------------|-------------|
| $\beta + 2e_k$ with $1 \leq k \leq 3$ | $(\beta_k + 2)(\beta_k + 1)T_{c_{2e_k}} [0]$ |
| $\beta + e_k + e_k'$ with $1 \leq k < k' \leq 3$ | $(\beta_k + 1)(\beta_{k'} + 1)T_{c_{e_k+e_{k'}}} [0]$ |
2.6 Construction of quasi-Trefftz functions

Given a point \( x_C \in \mathbb{R}^3 \) and a set of complex-valued functions \( c = \{ c_i, i \in \mathbb{N}_0^3, |i| \leq 2 \} \) satisfying Hypothesis 1, we can now turn back to the construction of solutions to Systems (7), (10) and (12), and hence the construction of quasi-Trefftz functions. Algorithm 1 summarizes one way to compute \( \xi = \{ \xi_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2 \} \) solution of a subsystem (13) for a given right hand side \( B^\ell \in \mathbb{C}; \beta \in (\mathbb{N}_0)^3, |\beta| = \ell \).

Remark 3. By deciding for a numbering scheme we broke the symmetry between the three component indices. Of course, under the assumption that \( T_{e_{\beta}e_1} [0] \neq 0 \), or \( T_{e_{\beta}e_2} [0] \neq 0 \), we could choose an index numbering scheme for which the corresponding matrix would have a similar echelon structure.

The space spanned by the \( \frac{(\ell+3)(\ell+4)}{2} \) columns of the matrix is of dimension \( \frac{(\ell+1)(\ell+2)}{2} \). The columns displaying a \( (\beta_1+2)(\beta_1+1)T_{e_{\beta}e_1} [0] \) entry form a linearly independent set, since they are in echelon form. Their indices are \( \{ \beta + 2e_1, \beta \in (\mathbb{N}_0)^3, |\beta| = \ell \} \), which is equivalent to \( \{ i \in (\mathbb{N}_0)^3, |i| = \ell + 2, i_1 > 1 \} \) as represented in Figure 2. Hence the indices of the remaining columns, i.e. the columns which do not display a \( (\beta_1+2)(\beta_1+1)T_{e_{\beta}e_1} [0] \) entry, are simply \( \{ i \in (\mathbb{N}_0)^3, |i| = \ell + 2, i_1 \leq 1 \} \).

Accordingly, for a given right hand side, we can take advantage of the echelon structure to compute a solution to the subsystem (13), by simply fixing first the values of the \( \{ \xi_i, i \in (\mathbb{N}_0)^3, |i| = \ell + 2, i_1 \leq 1 \} \) unknowns, and then solving by substitution the resulting square triangular system for the remaining unknowns \( \{ \xi_i, i \in (\mathbb{N}_0)^3, |i| = \ell + 2, i_1 > 1 \} \). See Algorithm 1.

2.6 Construction of quasi-Trefftz functions

Given a point \( x_C \in \mathbb{R}^3 \) and a set of complex-valued functions \( c = \{ c_i, i \in \mathbb{N}_0^3, |i| \leq 2 \} \) satisfying Hypothesis 1, we can now turn back to the construction of solutions to Systems (7), (10) and (12), and hence the construction of quasi-Trefftz functions. Algorithm 1 summarizes one way to compute \( \xi = \{ \xi_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2 \} \) solution of a subsystem (13) for a given right hand side \( B^\ell \in \mathbb{C}; \beta \in (\mathbb{N}_0)^3, |\beta| = \ell \).

Remarkably, Algorithms 2 to 4 build solutions to the non-linear problems (7), (10) and (12) while relying exclusively on explicit closed formulas.
Algorithm 1 $\xi = \text{solve subsystem} \left( \ell, B^\ell, \left\{ T_{c_{k+k'}} [0], 1 \leq k \leq k' \leq 3 \right\} \right)$

1: Fix $\{\xi_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2, i_1 \in \{0,1\}\}$
2: for $\beta_1 \leftarrow 0$ to $\ell$ do
3: for $\beta_2 \leftarrow 0$ to $\ell - \beta_1$ do
4: $\beta := (\beta_1, \beta_2, \ell - \beta_1 - \beta_2)$
5: $\xi_{\beta+2e_1} := \frac{1}{(\beta_1+2)(\beta_1+1)} \left( B^\ell - \sum_{k=2}^{3} (\beta_k + 2)(\beta_k + 1)T_{c_{2e_k}}[0] \xi_{\beta+2e_k} \right.$
6: $\left. - \sum_{1 \leq k < k' \leq 3} (\beta_k + 1)(\beta_{k'} + 1)T_{c_{k+k'}}[0] \xi_{\beta+e_k+e_{k'}} \right)$

Thanks to Algorithm 1, Algorithms 2 and 3 will compute a solution to systems (7) and (10) and then construct the associated GPWs $J$ and $G$, solutions to the initial problems (5) and (8), while Algorithm 4 will compute a solution to system (12) and construct the associated polynomial quasi-Trefftz function $H$.

Algorithm 2 Amplitude based

1: Given $x_C \in \mathbb{R}^3$, $q \in \mathbb{N}$ and $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ satisfying Hypothesis 1
2: Fix $\{\mu_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| \in \{0,1\}\}$ and $\Lambda \in \mathbb{C}^3$
3: for $\ell \leftarrow 0$ to $q - 1$ do
4: Compute $B^\ell = \{B^\ell_\beta \in \mathbb{C}; \beta \in (\mathbb{N}_0)^3, |\beta| = \ell\}$ according to
5: $B^\ell_\beta = - \sum_{\gamma < \beta} \sum_{k=1}^{3} T_{c_{2e_k}}[\beta - \gamma](\gamma_k + 2)(\gamma_k + 1)\mu_{\gamma+2e_k}$
6: $- \sum_{\gamma \leq \beta} \left( \sum_{k=1}^{3} T_{c_{2e_k}}[\beta - \gamma](2\Lambda_k(\gamma_k + 1)\mu_{\gamma+e_k} + \Lambda^2_k\mu_\gamma) \right.$
7: $\left. + \sum_{1 \leq k < k' \leq 3} T_{c_{e_k+e_{k'}}}[\beta - \gamma](\gamma_k + 1)(\gamma_{k'} + 1)\mu_{\gamma+e_k+e_{k'}} + \Lambda_k(\gamma_{k'} + 1)\mu_{\gamma+e_{k'}} \right.$
8: $\left. + \Lambda_{k'}(\gamma_k + 1)\mu_{\gamma+e_k} + \Lambda_k\Lambda_{k'}\mu_\gamma \right)$
9: $+ \sum_{k=1}^{3} T_{c_{e_k}}[\beta - \gamma](\gamma_k + 1)\mu_{\gamma+e_k} + \Lambda_k\mu_\gamma + T_{c_0}[\beta - \gamma] \mu_\gamma \right)$

5: Compute $\mu^\ell = \{\mu_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2\}$ via Algorithm 1
6: $\mu^\ell = \text{solve subsystem} \left( \ell, B^\ell, \left\{ T_{c_{k+k'}} [0], 1 \leq k \leq k' \leq 3 \right\} \right)$
7: $Q := \sum_{i \in \mathbb{N}_0^3, |i| \leq q+1} \mu_i X^i$ with $X^i = X_1^{i_1} X_2^{i_2} X_3^{i_3}$
8: $J(x) := Q(x - x_C) \exp \Lambda \cdot (x - x_C)$
Algorithm 3 Phase based

1: Given $x_C \in \mathbb{R}^3$, $q \in \mathbb{N}$ and $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ satisfying Hypothesis 1
2: Fix $\{\lambda_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| \in \{0, 1\}\}$
3: for $\ell \leftarrow 0$ to $q - 1$ do
4: Compute $B_\ell = \{B_\beta \in \mathbb{C}; \beta \in (\mathbb{N}_0)^3, |\beta| = \ell\}$ according to

$$B_\beta = -\sum_{\gamma<\beta} \sum_{k=1}^{3} T_{c_{2k}} [\beta - \gamma] (\gamma_k + 2)(\gamma_k + 1)\lambda_{\gamma+2e_k}$$

$$-\sum_{\gamma \leq \beta} \left( \sum_{k=1}^{3} T_{c_{2k}} [\beta - \gamma] \left( \sum_{\eta \leq \gamma} (\gamma_k - \eta_k + 1)\lambda_{\gamma-\eta+e_k} (\eta_k + 1)\lambda_{\eta+e_k} \right) + \sum_{1 \leq k < k' \leq 3} T_{c_{k+k'}} [\beta - \gamma] \left( (\gamma_k + 1)(\gamma_{k'} + 1)\lambda_{\gamma+e_k+e_{k'}} \right) + \sum_{\eta \leq \gamma} (\gamma_{k'} - \eta_k + 1)\lambda_{\gamma-\eta+e_{k'}}> 0 \right)\right) - T_{c_0}[\beta]$$

5: Compute $\lambda^\ell = \{\lambda_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2\}$ via Algorithm 1

$$\lambda^\ell = \text{solve subsystem} \left( \ell, B^\ell, \{T_{c_{k+k'}}[0], 1 \leq k \leq k' \leq 3\} \right)$$

6: $P := \sum_{i \in \mathbb{N}_0^3, |i| \leq q+1} \lambda_i X^i$ with $X^i = X_1^{i_1} X_2^{i_2} X_3^{i_3}$

7: $G(x) := \exp P(x - x_C)$
Algorithm 4 Polynomial

1: Given $x_C \in \mathbb{R}^3$, $q \in \mathbb{N}$ and $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ satisfying Hypothesis 1
2: Fix $\{\nu_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| \in \{0, 1\}\}$
3: for $\ell \leftarrow 0$ to $q - 1$ do
4: Compute $B^\ell = \{B^\ell_\beta \in \mathbb{C}; \beta \in (\mathbb{N}_0)^3, |\beta| = \ell\}$ according to

\[
B^\ell_\beta = -\sum_{\gamma<\beta} \sum_{k=1}^3 T_{c_{2\epsilon_k}}[\beta - \gamma](\gamma_k + 2)(\gamma_k + 1)\nu_{\gamma+2\epsilon_k} \\
-\sum_{\gamma\leq\beta} \left( \sum_{1\leq k\leq k'\leq 3} T_{c_{\epsilon_k+\epsilon_{k'}}}[\beta - \gamma](\gamma_k + 1)(\gamma_k' + 1)\nu_{\gamma+\epsilon_k+\epsilon_{k'}} \right. \\
+ \sum_{k=1}^3 T_{c_{\epsilon_k}}[\beta - \gamma](\gamma_k + 1)\nu_{\gamma+\epsilon_k} + T_{c_0}[\beta - \gamma]\nu_0 \right)
\]

5: Compute $\nu^\ell = \{\nu_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2\}$ via Algorithm 1

\[
\nu^\ell = \text{solve subsystem} \left( \ell, B^\ell, \{T_{c_{\epsilon_k+\epsilon_{k'}}}[0], 1 \leq k \leq k' \leq 3\} \right)
\]

6: $R := \sum_{i \in \mathbb{N}_0^3, |i| \leq q+1} \nu_i X^i$ with $X^i = X_1^{i_1}X_2^{i_2}X_3^{i_3}$

7: $H(x) := R(x-x_C)$

Interestingly, the quasi-Trefftz property of the quasi-Trefftz functions, $J$, $G$ and $H$, built from Algorithms 2 to 4 are satisfied independently of the fixed values throughout these algorithms: $\mathcal{L}_c J(x) = O(|x-x_C|^q)$, $\mathcal{L}_c G(x) = O(|x-x_C|^q)$ and $\mathcal{L}_c H(x) = O(|x-x_C|^q)$. We will refer to the choice of these values as the initialization process. However an appropriate choice of initialization will be crucial to prove approximation properties of the resulting sets of quasi-Trefftz functions.

### 2.7 Initialization

Keeping in mind the motivation for the design of GPWs, that is adding higher order terms either in the phase or the amplitude of a PW:

\[
(1 + \text{HOT}) \exp \Lambda \cdot \left( x - x_C \right) \text{ or } \exp \left[ \Lambda \cdot \left( x - x_C \right) + \text{HOT} \right],
\]

we now turn to the initialization process. From Algorithms 1 to 3 the free parameters in the construction of a GPW are $\{\lambda_i \in \mathbb{C} \text{ for } i \in (\mathbb{N}_0)^3, |i| \leq q+1, i_1 \in \{0, 1\}\}$ for a Phase-based GPW, and for an Amplitude-based GPW $\{\mu_i \in \mathbb{C} \text{ for } i \in (\mathbb{N}_0)^3, |i| \leq q+1, i_1 \in \{0, 1\}\}$ plus $\Lambda \in \mathbb{C}^3$. In both cases, we follow the intuition that lead to the choice of ansatz (15) as a generalization of PW functions to build a family of GPWs. In order to do so, only a few free parameters are sufficient, corresponding to the linear terms in the phase, and except for the constant coefficient of the amplitude for an Amplitude-based GPW, we will naturally set the remaining parameters to zero to reduce the amount of computation associated with the construction of each GPW. On the other hand, in the polynomial case, in order to prove the approximation properties of the resulting set of functions, besides the linear terms, we will also leverage the other free parameters to obtain a family of linearly independent quasi-Trefftz polynomials. To summarize,
Amplitude based | Phase-based | Polynomial | Comment
---|---|---|---
\(\Lambda \in \mathbb{C}^3\) | \(\{ \lambda_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = 1 \}\) | \(\{ \nu_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = 1 \}\) | \([1]\)
\(\mu_0\) | | \(\nu_0\) | Set to 1
\(\{ \mu_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = 1 \}\) | \(\lambda_0\) | | Set to 0

for \(\ell\) from 0 to \(q - 1\)
\(\{ \mu_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2, i_1 \in \{0, 1\} \}\) | for \(\ell\) from 0 to \(q - 1\)
\(\{ \lambda_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2, i_1 \in \{0, 1\} \}\) | Set to 0

for \(\ell\) from 0 to \(q - 1\)
\(\{ \nu_i \in \mathbb{C}; i \in (\mathbb{N}_0)^3, |i| = \ell + 2, i_1 \in \{0, 1\} \}\) | | \([2]\)

Initialization summary for the three types of quasi-Trefftz functions.

Top rows: corresponding to Step 1 in Algorithms [2] to [4]
Bottom rows: corresponding to Step 1 in Algorithm [1]

In order to completely define our choices of quasi-Trefftz functions, it is then sufficient to describe how are chosen: [1] the three parameters corresponding to linear terms, and [2] the other parameters in the polynomial case.

[1] In order to build not a single but rather a set of quasi-Trefftz functions, we now have three non-zero free parameters in each case, namely:

\[
\Lambda = \begin{bmatrix}
\Lambda_1 \\
\Lambda_2 \\
\Lambda_3
\end{bmatrix}
\begin{bmatrix}
\lambda_{e1} \\
\lambda_{e2} \\
\lambda_{e3}
\end{bmatrix}
\begin{bmatrix}
\nu_{e1} \\
\nu_{e2} \\
\nu_{e3}
\end{bmatrix}
\in \mathbb{C}^3,
\]

(16)

In the constant-coefficient Helmholtz case, the matrix \(\mathcal{C}\) introduced in Hypothesis [1] is the identity \(I_3\) and it is then natural to fix these as \(sd\), with \(s = i\), to obtain a PW exact solution since \((sd)^T(I_3sd) = -\kappa^2\) is independent of \(d\). Yet in the general case, this matrix \(\mathcal{C}\) is associated with anisotropy in the second order terms of the partial differential operator, and it is then natural to introduce (i) the orthonormal basis of eigenvectors of \(\mathcal{C}\) via \(P\) and (ii) the anisotropic scaling by the eigenvalues of \(\mathcal{C}\) via \(D\). Hence for each quasi-Trefftz function, under Hypothesis [1] we will fix these as \(s^{PD^{-1/2}}d\), where \(s \in \mathbb{C}^*\) and \(d \in \mathbb{R}^3\) with \(|d| = 1\). To define a set of \(p\) distinct – and linearly independent as we will see later – quasi-Trefftz functions, we will choose distinct directions \(\{d_l \in \mathbb{R}^3\text{ for } l\text{ from }1\text{ to }p; |d_l| = 1\text{ with }d_{L} \neq d_k \text{ if } k \neq l\}\) while we will choose a common value for \(s\) for each of the \(p\) functions in the set. Each direction \(d_l\) will be defined by two angles \((\theta_l, \phi_l)\) as follows:

\[
d_l = \begin{bmatrix}
\sin \theta_l \sin \phi_l \\
\sin \theta_l \cos \phi_l \\
\cos \theta_l
\end{bmatrix}.
\]

Under Hypothesis [1] for any \(X = s^{PD^{-1/2}}d\), we can easily verify that:

\[
X^T(\mathcal{C}X) = s^2(\mathcal{P}D^{-1/2}d)^T(\mathcal{P}D\mathcal{P}^T)(\mathcal{P}D^{-1/2}d)
= s^2d^Td
= s^2,
\]

or equivalently:

\[
\sum_{k=1}^{3} T_{c_{ek}}[0] (X_k)^2 + \sum_{1 \leq k < k' \leq 3} T_{c_{ek} + c_{ek'}}[0]X_k'X_k = s^2.
\]
As a result, this quantity does not depend on the direction \( d \), but rather has the same value for the whole set of functions, as we discussed in the Helmholtz case. This crucial fact will be key to prove approximation properties of the quasi-Trefftz functions.

**Remark 4.** As a result of this choice, the GPW functions boil down to classical PWs in the case of a constant coefficient Helmholtz equation.

\[ \text{(17)} \]

This particular choice will allow us to prove approximation properties of the corresponding polynomial quasi-Trefftz basis.

### 3 Approximation properties

The construction of quasi-Trefftz functions is based on Taylor expansions, it is therefore natural to use similar tools to study their approximation properties. The central idea here is precisely to approximate a given exact PDE solution \( u \) by a linear combination \( u_a \) of quasi-Trefftz functions by matching their respective Taylor expansions at \( x_C \). Indeed, for any order of approximation \( n \), we have:

\[
\forall i \in (\mathbb{N}_0)^3, |i| \leq n, \quad \partial_i u(x_C) = \partial_i u_a(x_C), \quad \Rightarrow u_a(x) - u(x) = O\left(|x - x_C|^{n+1}\right). \tag{18}
\]

This in turn leads to the convergence of \( u - u_a \) in various norms of interest in the regime \( |x - x_C| \to 0 \), moreover higher order convergence follows from increasing the value of the order of approximation \( n \) in the Taylor expansion.

Matching the Taylor expansion of a linear combination \( u_a \) of quasi-Trefftz functions to that of a given function \( u \) leads to a linear system.

- Each unknown is a weight of the desired linear combination, and is indexed \( l \); there are as many unknowns as there are functions in the quasi-Trefftz set.

- Each equation corresponds to one Taylor expansion coefficient, and is indexed \( i \in (\mathbb{N}_0)^3 \) with \( |i| \leq n \); there are \((n+1)(n+2)(n+3)/6\) equations.

The system’s matrix can then be defined for a given list of quasi-trefftz function thanks to a numbering of the equations. The entries of the system’s matrix are the partial derivatives of quasi-Trefftz functions evaluated at \( x_C \). Hence, given any numbering of multi-indices \( N \), for any family of \( p \) functions \( \{b_l, \text{ for } l \in \mathbb{N}, l \leq p\} \), the \((N(i),l)\) entry of the corresponding \( n \times p \) matrix \( M^{n,p}_{N,i} \) is:

\[
M^{n,p}_{N(i),l} = \frac{\partial_i^l b_l(x_C)}{i!} = T_{b_l}[i] \tag{19}
\]

Moreover, the value \( p = (n+1)^2 \) will be of particular interest in what follows. So to simplify the notation, the matrix corresponding to \( p = (n+1)^2 \) will be denoted with the superscript \([n]\), for instance \( M^{[n]} \) instead of \( M^{n,(n+1)^2} \). For three families of quasi-Trefftz functions introduced in the previous section, we will use the following notation for the corresponding matrices.

| Amplitude-based functions | Phase-based functions | Polynomial functions |
|-------------------------|----------------------|---------------------|
| \( A^{n,p} \) and \( A^{[n]} \) | \( P^{n,p} \) and \( P^{[n]} \) | \( Q^{n,p} \) and \( Q^{[n]} \) |
In order to evidence the structure of the linear system, the equations will be numbered as follows. To leverage the loop structure of Algorithms 2 to 4, we want $N$ to satisfy $|i| < |j|$ implies that $N(i) < N(j)$, hence we write it as:

$$\forall i \in (N_0)^3 \text{ with } |i| \leq n, N(i) = \frac{|i|(|i| + 1)(|i| + 2)}{6} + N_{ii}(i),$$

for some $N_m$ providing a numbering of indices of length $m$. For instance we can choose $N_m$ to count indices according to the linear order $\preceq$ within the level $m$ and in this case the numbering corresponds to $N(i) = \sum_{j < i} 1$, or choose $N_m(i) = (i2 + i3)(i2 + i3 + 1)/2 + i3 + 1$ for all $i$ such that $|i| = m$.

A road map was proposed in [24] to prove approximation properties of quasi-Trefftz functions. It can be summarized as follows:

1. for each quasi-Trefftz function, express all the basic parameters in Algorithms 2 to 4 in terms of the free parameters that are not set to 0;
2. identify a reference case, here a classical PW case;
3. study useful properties of the reference matrix;
4. establish a link between each of the quasi-Trefftz cases and the reference case;
5. prove the approximation properties of quasi-Trefftz bases.

While Items 2, 3 and 5 are case-independent, Items 1 and 4 will be treated separately for each family of quasi-Trefftz functions. These two key points rely on understanding how the entries of the linear system matrices depend on the initialization of our quasi-Trefftz functions, emphasizing their properties shared by corresponding entries on a given row as well as their differences. Two important questions about these matrices concern their rank. (i) How large of a rank can they have? (ii) What particular choice of angles in the initialization parameters can guarantee the maximal rank? These will lead the choice (i) of how many different quasi-Trefftz functions to define, and (ii) of how to choose the initialization angles. As a by-product, the resulting families of quasi-Trefftz functions will be proved to be linearly independent.

Given an order $n$ for the approximation property (18), the order $q$ of the quasi-Trefftz property will be chosen to guarantee a similar construction for all the polynomial coefficients of quasi-Trefftz basis functions that will appear in the Taylor expansion (18). This will require to set $q \geq n - 1$, it is then sufficient to construct the quasi-Trefftz basis functions with the parameter $q$ satisfying:

$$q = \max(n - 1, 1)$$

This will be particularly helpful to describe all polynomial coefficients of the quasi-Trefftz basis functions in terms of the initialization parameters, see Section 3.4.

It seems important to underline the fundamental part that the interplay of Hypothesis 1 and the choice of initialization will play in the rest of this section.

### 3.1 Preliminary results

The goal is to investigate how the terms computed in Algorithms 1 to 3, namely $\mu_{\beta + 2e_1}$ and $\lambda_{\beta + 2e_1}$, depend on the three free parameters from the initialization process (16). We will proceed by induction with respect to the level $\ell$. In each case the result will rely on a careful inspection of the right-hand side $B^\ell$ of the subsystems.
3.1.1 For amplitude-based GPWs

For an amplitude-based GPW, we focus on investigating properties of \( \{\mu_i \in \mathbb{C}, i \in \mathbb{N}_0^3, |i| \leq q + 1\} \). Here, the three non-zero free parameters in the initialization procedure are \( \Lambda_1, \Lambda_2, \Lambda_3 \). All \( \mu \)s computed from Algorithms 1 and 2 clearly appear to be polynomials with respect to these three free parameters, that is they are elements of \( \mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3] \). Moreover, as first noted in [15], the initialization ensures that

\[
Q_N = 0, \quad \text{where } Q_N(\Lambda_1, \Lambda_2, \Lambda_3) := \sum_{k=1}^{3} T_{c_{2 e_k}}[0] (\Lambda_k)^2 + \sum_{1 \leq k < k' \leq 3} T_{c_{e_k + e_{k'}}}[0] \Lambda_k \Lambda_{k'} - s^2
\]

which turns our attention to elements of \( \mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3]/(Q_N) \) instead. We will therefore investigate how the other \( \mu \)s can be expressed in terms of the three free parameters, \( \Lambda_1, \Lambda_2, \Lambda_3 \).

**Lemma 1.** Given \( q \in \mathbb{N} \), a point \( x_C \in \mathbb{R}^3 \), a set of complex-valued functions \( c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\} \) is assumed to satisfy Hypothesis [7].

Consider any amplitude-based GPW associated to differential operator \( L_c \), \( J(x) := Q(x - x_C) \exp \Lambda \cdot (x - x_C) \) with \( Q := \sum_{i \in \mathbb{N}_0^3, |i| \leq q+1} \mu_i X^i \), constructed via Algorithms 1 and 2 with the initialization introduced in Section 2.7 for \( s \in \mathbb{C}^* \) a unit vector \( d \in \mathbb{S}^2 \). Then \( \mu_{2e_1} \) can be expressed as a polynomial of degree at most equal to 1 in \( \mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3] \), with coefficients depending on \( s \) yet independent of \( d \).

**Proof.** From the formulas in Algorithms 1 and 2 for \( \ell = 0 \) and \( \beta = 0 \) we get:

\[
\begin{align*}
\mu_{2e_1} &= \frac{1}{2 T_{c_{2e_1}}[0]} \left( B_0^0 - \sum_{k=1}^{3} 2 T_{c_{2e_k}}[0] \mu_{2e_k} - \sum_{1 \leq k < k' \leq 3} T_{c_{e_k + e_{k'}}}[0] \mu_{e_k + e_{k'}} \right), \\
B_0^0 &= -\sum_{k=1}^{3} T_{c_{2e_k}}[0] (2 \Lambda_k \mu_{e_k} + \Lambda_k^2 \mu_0) - \sum_{1 \leq k < k' \leq 3} T_{c_{e_k + e_{k'}}}[0] (\Lambda_k \mu_{e_k} + \Lambda_{k'} \mu_{e_k} + \Lambda_k \Lambda_{k'} \mu_0) \\
&- \sum_{k=1}^{3} T_{c_{e_k}}[0] \mu_{e_k} + \Lambda_k \mu_0 - T_{c_0}[0] \mu_0,
\end{align*}
\]

so the initialization implies:

\[
\begin{align*}
\mu_{2e_1} &= \frac{1}{2 T_{c_{2e_1}}[0]} B_0^0, \\
B_0^0 &= -\sum_{k=1}^{3} T_{c_{2e_k}}[0] \Lambda_k^2 - \sum_{1 \leq k < k' \leq 3} T_{c_{e_k + e_{k'}}}[0] \Lambda_k \Lambda_{k'} - \sum_{k=1}^{3} T_{c_{e_k}}[0] \Lambda_k - T_{c_0}[0], \\
&= -Q_N(\Lambda_1, \Lambda_2, \Lambda_3) - s^2 - \sum_{k=1}^{3} T_{c_{e_k}}[0] \Lambda_k - T_{c_0}[0],
\end{align*}
\]

Therefore, since \( Q_N(\Lambda_1, \Lambda_2, \Lambda_3) = 0 \), we obtain

\[
\mu_{2e_1} = \frac{1}{2 T_{c_{2e_1}}[0]} \left( -s^2 - \sum_{k=1}^{3} T_{c_{e_k}}[0] \Lambda_k - T_{c_0}[0] \right),
\]

which proves the claim since \( s \) is a fixed constant according to the initialization. \( \square \)

**Proposition 1.** Given \( q \in \mathbb{N} \) and a point \( x_C \in \mathbb{R}^3 \), a set of complex-valued functions \( c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\} \) is assumed to satisfy Hypothesis [7].

Consider any amplitude-based GPW, \( J(x) := Q(x - x_C) \exp \Lambda \cdot (x - x_C) \) with \( Q := \sum_{i \in \mathbb{N}_0^3, |i| \leq q+1} \mu_i X^i \), constructed via Algorithms 1 and 2 with the initialization introduced in Section 2.7 for \( s \in \mathbb{C}^* \) a unit vector...
\( \mathbf{d} \in \mathbb{S}^2 \). Then, for all \( \ell \) from 0 to \( q - 1 \) and all \( \beta \in (\mathbb{N}_0)^3 \) such that \( |\beta| = \ell \), \( \mu_{\beta + 2e_1} \) can be expressed as a polynomial of degree at most equal to \( |\beta| + 1 \) in \( \mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3] \), with coefficients depending on \( \mathbf{s} \) yet independent of \( \mathbf{d} \).

**Proof.** We will proceed by induction with respect to \( \mu_{\beta + 2e_1} \) terms are computed in the algorithms.

The case \( \beta = 0 \) is precisely Lemma 1.

Assume \( \beta \in (\mathbb{N}_0)^3 \) with \( 0 < \beta \) is such that the result holds for all \( \beta' < \beta \): \( \mu_{\beta' + 2e_1} \) can be expressed as a polynomial of degree at most equal to \( |\beta'| + 1 \) in \( \mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3] \). Then \( \mu_{\beta + 2e_1} \) is computed according to Algorithms 1 and 2. Hence, since

\[
2\Lambda_k(\gamma_k + 1)\mu_{1 + e_k} + \Lambda_k^2\mu_{2} = \Lambda_k(\gamma_k' + 1)\mu_{1 + e_k} + \Lambda_k(\gamma_k + 1)\mu_{1 + e_k} + \Lambda_k\Lambda_k'\mu_{2} \quad \text{for } k' = k,
\]

we can gather these terms in a sum over \( 1 \leq k \leq k' \leq 3 \) and \( \mu_{\beta + 2e_1} \) can be written as:

\[
\mu_{\beta + 2e_1} = \frac{1}{(\beta + 2)(\beta + 1)T_{\mathbf{c}_{2\mathbf{e}_1}}} [0] \left( -\sum_{\gamma < \beta} \sum_{k=1}^3 T_{\mathbf{c}_{2\mathbf{e}_k}} [\beta - \gamma](\gamma_k + 2)(\gamma_{k'} + 1)\mu_{1 + e_k} \right.
\]

\[
- \sum_{\gamma \leq \beta} \sum_{1 \leq k' < 3} T_{\mathbf{c}_{2\mathbf{e}_k}} [\beta - \gamma](\gamma_k + 1)(\gamma_{k'} + 1)\mu_{1 + e_k + e_{k'}}
\]

\[
- \sum_{\gamma \leq \beta} \sum_{1 \leq k' < 3} T_{\mathbf{c}_{2\mathbf{e}_k}} [\beta - \gamma]\left( \Lambda_k(\gamma_k + 1)\mu_{1 + e_k} + \Lambda_k(\gamma_{k'} + 1)\mu_{1 + e_{k'}} + \Lambda_k\Lambda_k'\mu_{2} \right)
\]

\[
- \sum_{\gamma \leq \beta} \left( \sum_{k=1}^3 T_{\mathbf{c}_{2\mathbf{e}_k}} [\beta - \gamma](\gamma_k + 1)\mu_{1 + e_k} + \Lambda_k\mu_{2} \right) + T_{\mathbf{c}_0} [\beta - \gamma] \mu_{2} \right)
\]

\[
- \sum_{k=2}^3 (\beta_k + 2)(\gamma_k + 1)T_{\mathbf{c}_{2\mathbf{e}_k}} [0] \mu_{1 + 2e_k}
\]

\[
- \sum_{1 \leq k < k' \leq 3} (\beta_k + 1)(\beta_{k'} + 1)T_{\mathbf{c}_{2\mathbf{e}_k + e_{k'}}} [0] \mu_{1 + e_k + e_{k'}}
\).
\]

On the right hand side we observe that the \( \mu \) terms fall in one of two categories as elements of \( \mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3] \):

1. \( \mu_i \) with \( i_1 \in \{0, 1\} \), chosen in the initialization process, either \( \mu_0 = 1 \) or otherwise the terms set to zero,

2. \( \mu_i \) with \( i_1 \geq 2 \), computed at a previous iteration for \( \beta' = i - 2e_1 \prec \beta \).

The linear terms can be listed as follows.
\[ \begin{array}{|c|l|l|l|} \hline \text{Terms} & \text{Indices} & 0 & 1 & \mu_{\beta'+2e_1} \\
\hline \mu_{\gamma+2e_k} & \gamma < \beta(\neq 0), k \in \{1, 2, 3\} & & & \checkmark \\
 & (\gamma + 2e_k)_1 \in \{0, 1\} & & & \\
\hline \mu_{\gamma+2e_k} & \gamma < \beta(\neq 0), k \in \{1, 2, 3\} & & \beta' = \gamma + 2(e_k - e_1) & \\
 & (\gamma + 2e_k)_1 > 1 & & & \\
\hline \mu_{\gamma+e_k+e_{k'}} & \gamma \leq \beta, 1 \leq k < k' \leq 3 & & & \checkmark \\
 & (\gamma + e_k + e_{k'})_1 \in \{0, 1\} & & & \\
\hline \mu_{\gamma+e_k+e_{k'}} & \gamma \leq \beta, 1 \leq k < k' \leq 3 & & \beta' = \gamma + e_k + e_{k'} - 2e_1 & \\
 & (\gamma + e_k + e_{k'})_1 > 1 & & & \\
\hline \mu_{\gamma+e_k} & \gamma \leq \beta, k \in \{1, 2, 3\} & & \beta' = \gamma + e_k - 2e_1 & \\
 & (\gamma + e_k)_1 \in \{0, 1\} & & & \\
\hline \mu_{\gamma} & \gamma = 0 & & & \checkmark \\
\hline \mu_{\gamma} & \gamma \leq \beta & & & \checkmark \\
 & (\gamma)_1 \in \{0, 1\}, \gamma \neq 0 & & & \\
\hline \mu_{\beta+2e_k} & k \in \{2, 3\} & & \beta' = \gamma - 2e_1 & \\
 & (\beta + 2e_k)_1 \in \{0, 1\} & & & \\
\hline \mu_{\beta+2e_k} & k \in \{2, 3\} & & \beta' = \beta + 2(e_k - e_1) & \\
 & (\beta + 2e_k)_1 > 1 & & & \\
\hline \mu_{\beta+e_k+e_{k'}} & 1 \leq k < k' \leq 3 & & \beta' = \beta + e_k + e_{k'} - 2e_1 & \\
 & (\beta + e_k + e_{k'})_1 \in \{0, 1\} & & & \\
\hline \end{array} \]

Hence the linear terms can be expressed as elements of \(\mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3]\) as either 0, 1, or by induction hypothesis as a polynomial of degree at most equal to \(|\beta'| + 1\). Moreover, in this last case, the values of \(\beta'\) identified in the previous table are such that:

\[
\begin{cases}
\gamma < \beta \Rightarrow |\gamma + 2(e_k - e_1)| + 1 < |\beta| + 1, \\
\gamma \leq \beta \Rightarrow |\gamma + e_k + e_{k'} - 2e_1| + 1 \leq |\beta| + 1, \\
\gamma \leq \beta \Rightarrow |\gamma + e_k - 2e_1| + 1 \leq |\beta|,
\end{cases}
\]

and

\[
\begin{cases}
|\beta + 2(e_k - e_1)| + 1 = |\beta| + 1, \\
|\beta + e_k + e_{k'} - 2e_1| + 1 = |\beta| + 1.
\end{cases}
\]

In summary all the linear terms in the right hand side of (20) can be expressed as polynomials of degree at most equal to \(|\beta| + 1\) in \(\mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3]\).

As for the non-linear terms, they all appear for indices \(\gamma \leq \beta\) and \(1 \leq k \leq k' \leq 3\), and they can be identified as follows.
For a phase-based GPW, we focus on investigating properties of $H$ hence as elements of $C[\Lambda_1, \Lambda_2, \Lambda_3]$, these non-linear terms can be expressed either as zero or by induction hypothesis as a polynomial of degree at most equal to:

- $|\beta'| + 2 \leq |\beta|$ in cases 1 and 2,
- $2$ in case 3,
- $|\beta'| + 3 \leq |\beta| + 1$ in case 4,
- $1$ in case 5,
- $|\beta'| + 2 \leq |\beta|$ in case 6.

In summary all the non-linear terms in the right hand side of (20) can be expressed as polynomials of degree at most equal to $|\beta| + 1$ in $C[\Lambda_1, \Lambda_2, \Lambda_3]$.

Therefore $\mu_{\beta'+2e_1}$ in (20) can be expressed as a polynomial of degree at most equal to $|\beta| + 1$ in $C[\Lambda_1, \Lambda_2, \Lambda_3]$. This concludes the proof.

### 3.1.2 For phase-based GPWs

For a phase-based GPW, we focus on investigating properties of $\{\lambda_i \in \mathbb{C}, i \in \mathbb{N}_0^3, |i| \leq q + 1\}$. Here, the three non-zero free parameters in the initialization procedure are $\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}$. All $\lambda$s computed from Algorithms 1 and 3 clearly appear to be polynomials with respect to these three free parameters, that is they are elements of $C[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]$. Moreover, as first noted in [18], the initialization ensures that

$$P_N = 0, \text{ where } P_N(\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}) := \sum_{k=1}^{3} T_{c_{2e_k}[0]}(\lambda_{e_k})^2 + \sum_{1 \leq k < k' \leq 3} T_{c_{e_k+e_{k'}}[0]}\lambda_{e_k}\lambda_{e_{k'}} - s^2$$

which turns our attention to elements of $C[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]/(P_N)$ instead. We will therefore investigate how the other $\lambda$s can be expressed in terms of the three free parameters, $\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}$.

**Lemma 2.** Given $q \in \mathbb{N}$ and a point $x_C \in \mathbb{R}^3$, a set of complex-valued functions $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ is assumed to satisfy Hypothesis [1]

Consider any phase-based GPW associated to the partial differential operator $L_c$, $G(x) := \exp P(x - x_C)$ with $P := \sum_{i \in \mathbb{N}_0^3, |i| \leq q+1} \lambda_i X^i$, constructed via Algorithms 1 and 3 with the initialization introduced in Section 2.7 for $s \in \mathbb{C}^*$ and a unit vector $d$. Then $\lambda_{2e_1}$ can be expressed as a polynomial of degree at most equal to 1 in $C[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]$, with coefficients depending on $s$ yet independent of $d$. 

| Terms | Indices | 0 | 1 | $\Lambda_k$ or $\Lambda_k'$ | $\mu_{\beta'+2e_1}$ | Case |
|-------|---------|---|---|-----------------|-----------------|-----|
| $\Lambda_k \mu_{e_1}^\gamma$ | $(\gamma + e_1_1) \in \{0, 1\}$ | ✓ | ✓ | ✓ | ✓ | 1 |
| $\Lambda_k \mu_{e_1}^\gamma$ | $(\gamma + e_1_1) > 1$ | ✓ | ✓ | ✓ | ✓ | 2 |
| $\Lambda_k \mu_{e_1}^\gamma$ | $(\gamma + e_1_1) \in \{0, 1\}$ | ✓ | ✓ | ✓ | ✓ | 3 |
| $\Lambda_k \mu_{e_1}^\gamma$ | $(\gamma) > 1$ | ✓ | ✓ | ✓ | ✓ | 4 |
| $\Lambda_k \mu_{e_1}^\gamma$ | $(\gamma) \in \{0, 1\}, \gamma \neq 0$ | ✓ | ✓ | ✓ | ✓ | 5 |
| $\Lambda_k \mu_{e_1}^\gamma$ | $(\gamma) > 1$ | ✓ | ✓ | ✓ | ✓ | 6 |
Proof. Since $\lambda_{2e_1}$ is computed at iteration $\ell = 0$ in Algorithm 3 according to Algorithm 1, we have:

$$\lambda_{2e_1} = \frac{1}{2T_{c2e_1}} \left( B^0_0 - \sum_{k=2}^{3} 2T_{c2e_k} [0] \lambda_{2e_k} - \sum_{1 \leq k < k' \leq 3} T_{c_{k+k'}} [0] \lambda_{e_k + e_{k'}} \right),$$

so the initialization then implies:

$$\lambda_{2e_1} = \frac{1}{2T_{c2e_1}} B^0_0,$$

(21)

By definition, the right hand side $B^0_0 = [B^0_0] \in \mathbb{C}$ is:

$$B^0_0 = -\sum_{k=1}^{3} T_{c_{2e_k}} [0] (\lambda_{e_k})^2 - \sum_{1 \leq k < k' \leq 3} T_{c_{k+k'}} [0] \left( \lambda_{e_k + e_{k'}} + \lambda_{e_{k'}}, \lambda_{e_k} \right) - \sum_{k=1}^{3} T_{c_k} [0] \lambda_{e_k} - T_{c_0} [0],$$

$$= -P_N(\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}) - s^2 - \sum_{1 \leq k < k' \leq 3} T_{c_{k+k'}} [0] \lambda_{e_k + e_{k'}} - \sum_{k=1}^{3} T_{c_k} [0] \lambda_{e_k} - T_{c_0} [0],$$

so from the initialization, imposing all the $\lambda_{e_k + e_{k'}}$ to be zero as well as $P_N = 0$, we can express the right hand side as:

$$B^0_0 = -s^2 - \sum_{k=1}^{3} T_{c_k} [0] \lambda_{e_k} - T_{c_0} [0].$$

(22)

As a result, combining (21) and (22) yields:

$$\lambda_{2e_1} = \frac{1}{2T_{c2e_1}} \left( -s^2 - \sum_{k=1}^{3} T_{c_k} [0] \lambda_{e_k} - T_{c_0} [0] \right),$$

which proves the claim since $s$ is a fixed constant according to the initialization. \qed

Proposition 2. Given $q \in \mathbb{N}$ and a point $x_C \in \mathbb{R}^3$, a set of complex-valued functions $c = \{ c_i, i \in \mathbb{N}_0^3, |i| \leq 2 \}$ is assumed to satisfy Hypothesis 4.

Consider any phase-based GPW associated to the partial differential operator $L_c$, $G(x) := \exp P(x - x_C)$ with $P := \sum_{i \in \mathbb{N}_0^3, |i| \leq q + 1} \lambda_i x^i$, constructed via Algorithms 4 and 3 with the initialization introduced in Section 2.7 for $s \in \mathbb{C}^*$ and a unit vector $d$. Then, for all $\ell$ from 0 to $q - 1$ and all $\beta \in (\mathbb{N}_0)^3$ such that $|\beta| = \ell$, $\lambda_{\beta + 2e_1}$ can be expressed as a polynomial of degree at most equal to $|\beta| + 1$ in $\mathbb{C}[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]$, with coefficients depending on $s$ yet independent of $d$.

Proof. We will proceed by induction with respect to $\beta$ according to the linear order $\prec$, which corresponds to the order in which the $\lambda_{\beta + 2e_k}$ terms are computed in the algorithms.

The case $\beta = 0$ is precisely Lemma 2.

Assume $\beta \in (\mathbb{N}_0)^3$ with $0 \prec \beta$ is such that the result holds for all $\beta' \prec \beta$: $\lambda_{\beta' + 2e_1}$ can be expressed as a polynomial of degree at most equal to $|\beta'| + 1$ in $\mathbb{C}[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]$. Then $\lambda_{\beta + 2e_1}$ is computed according to Algorithms 4 and 3. Hence, since

$$(\gamma_k - \eta_k + 1)\lambda_{\gamma - \eta + e_k} (\eta_k + 1)\lambda_{\eta + e_k} = (\gamma_k' - \eta_k' + 1)\lambda_{\gamma - \eta + e_{k'}} (\eta_k + 1)\lambda_{\eta + e_k}$$

for $k' = k,$

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we can gather these terms in a sum over $1 \leq k \leq k' \leq 3$ and $\lambda_{\beta+2e_1}$ can be written as:

$$\lambda_{\beta+2e_1} = \frac{1}{(\beta_1 + 2)(\beta_1 + 1)T_{c_2e_1} [0]} \left( - \sum_{\gamma < \beta, k}^{3} \sum_{k=1}^{3} T_{c_2e_k} [\beta - \gamma] (\gamma_k + 2)(\gamma_k + 1)\lambda_{\gamma+2e_k} \right.$$

$$\left. - \sum_{\gamma < \beta, 1 \leq k < k' \leq 3} T_{c_2e_{k+k'}} [\beta - \gamma] (\gamma_k + 1)(\gamma_k + 1)\lambda_{\gamma+e_k+e_{k'}} \right.$$  

$$\left. - \sum_{\gamma < \beta, 1 \leq k < k' \leq 3} T_{c_2e_k} [\beta - \gamma] (\gamma_k - \eta_k + 1)\lambda_{\gamma-\eta+e_k} (\eta_k + 1)\lambda_{\eta+e_k} \right.$$  

$$\left. - \sum_{\gamma < \beta, k = 1}^{3} (\beta_k + 2)(\beta_k + 1)T_{c_2e_k} [0]\lambda_{\beta+2e_k} \right)$$  

(23)

On the right hand side we observe that the $\lambda$ terms fall in one of two categories as elements of $\mathbb{C}[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]$:

1. $\lambda_i$ with $i_1 \in \{0, 1\}$, chosen in the initialization process, either a $\lambda_{e_k}$ or otherwise the terms set to zero,

2. $\lambda_i$ with $i_1 \geq 2$, computed at a previous iteration for $\beta' = i - 2e_1 < \beta$.

The linear terms can be listed as follows.

| Terms | Indices | 0 $\lambda_{e_k}$ | $\lambda_{\beta'+2e_1}$ |
|-------|---------|------------------|---------------------|
| $\lambda_{\gamma+2e_k}$ | $\gamma < \beta(\neq 0), k \in \{1, 2, 3\}$ | ✓ | ✓ |
| $\lambda_{\gamma+e_k}$ | $\gamma < \beta(\neq 0), k \in \{1, 2, 3\}$ | ✓ | ✓ |
| $\lambda_{\gamma+e_{k+k'}}$ | $\gamma \leq \beta, 1 \leq k < k' \leq 3$ | ✓ | ✓ |
| $\lambda_{\gamma+e_k+e_{k'}}$ | $\gamma \leq \beta, 1 \leq k < k' \leq 3$ | ✓ | ✓ |
| $\lambda_{\gamma+e_k}$ | $\gamma = 0, k \in \{1, 2, 3\}$ | ✓ | ✓ |
| $\lambda_{\gamma+e_k}$ | $\gamma \leq \beta, k \in \{1, 2, 3\}$ | ✓ | ✓ |
| $\lambda_{\beta+2e_k}$ | $k \in \{2, 3\}$ | ✓ | ✓ |
| $\lambda_{\beta+2e_k}$ | $k \in \{2, 3\}$ | ✓ | ✓ |
| $\lambda_{\beta+e_k+e_{k'}}$ | $1 \leq k < k' \leq 3$ | ✓ | ✓ |
| $\lambda_{\beta+e_k+e_{k'}}$ | $1 \leq k < k' \leq 3$ | ✓ | ✓ |

Hence the linear terms can be expressed as elements of $\mathbb{C}[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]$ as either 0, or a $\lambda_{e_k}$, or by induction hypothesis as a polynomial of degree at most equal to $|\beta'| + 1$. Moreover, in this last case, the values of $\beta'$
identified in the previous table are such that:

\[
\begin{align*}
\gamma < \beta & \Rightarrow |\gamma + 2(e_k - e_1)| + 1 < |\beta| + 1, \\
\gamma \leq \beta & \Rightarrow |\gamma + e_k + e_{k'} - 2e_1| + 1 \leq |\beta| + 1, \\
\gamma \leq \beta & \Rightarrow |\gamma + e_k - 2e_1| + 1 \leq |\beta|, \\
\end{align*}
\]

and

\[
\begin{align*}
|\beta + 2(e_k - e_1)| + 1 & = |\beta| + 1, \\
|\beta + e_k + e_{k'} - 2e_1| + 1 & = |\beta| + 1, \\
|\beta + e_k + e_{k'} - 2e_1| + 1 & = |\beta| + 1.
\end{align*}
\]

In summary all the linear terms in the right hand side of (23) can be expressed as polynomials of degree at most equal to $|\beta| + 1$ in $\mathbb{C}[^{\lambda}{\lambda}_1, ^{\lambda}{\lambda}_2, ^{\lambda}{\lambda}_3]$.

As for the non-linear terms, all of the form $\lambda_{\gamma - \eta + e_{k'}}\lambda_{\eta + e_k}$ with $\eta \leq \gamma \leq \beta$, they can be described as follows.

| Indices | $0$ | $\lambda_{e_k}$ or $\lambda_{e_{k'}}$ | $\lambda_{\beta' + 2e_1}$ |
|---|---|---|---|
| $\eta = \gamma = 0$ | ✓ | ✓ | |
| $\eta = 0, \gamma \neq 0$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |
| $(\gamma - \eta + e_{k'})_1 \in \{0, 1\}$ | ✓ | ✓ | $\beta' = \eta + e_k - 2e_1$ |
| $\eta = 0$ | ✓ | ✓ | $\beta' = \eta + e_k - 2e_1$ |
| $(\gamma - \eta + e_{k'})_1 > 1$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |
| $\eta \neq 0$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |
| $(\eta + e_k)_1 \in \{0, 1\}$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |
| $\eta = \gamma$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |
| $(\eta + e_k)_1 > 1$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |
| $(\gamma - \eta + e_{k'})_1 \in \{0, 1\}$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |
| $(\eta + e_k)_1 > 1$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |
| $(\gamma - \eta + e_{k'})_1 > 1$ | ✓ | ✓ | $\beta' = \gamma + e_{k'} - 2e_1$ |

Hence the non-linear terms can be expressed as elements of $\mathbb{C}[^{\lambda}{\lambda}_1, ^{\lambda}{\lambda}_2, ^{\lambda}{\lambda}_3]$ as either 0, or a $\lambda_{e_k}\lambda_{e_{k'}}$, or by induction hypothesis as a polynomial of degree at most equal to $|\beta'| + 2$ or $|\beta'| + |\beta''| + 2$. Moreover, in this last two cases, the values of $\beta'$ and $\beta''$ identified in the previous table are such that:

\[
\begin{align*}
\gamma \leq \beta & \Rightarrow |\gamma + e_{k'} - 2e_1| + 2 \leq |\beta| + 1 \\
\eta \leq \beta & \Rightarrow |\eta + e_k - 2e_1| + 2 \leq |\beta| + 1 \\
\gamma \leq \beta & \Rightarrow |\eta + e_k - 2e_1| + |\gamma - \eta + e_{k'} - 2e_1| + 2 \leq |\beta|
\end{align*}
\]

In summary all the non-linear terms in the right hand side of (23) can be expressed as polynomials of degree at most equal to $|\beta| + 1$ in $\mathbb{C}[^{\lambda}{\lambda}_1, ^{\lambda}{\lambda}_2, ^{\lambda}{\lambda}_3]$.

Therefore $\lambda_{\beta + 2e_1}$ in (23) can be expressed as a polynomial of degree at most equal to $|\beta| + 1$ in $\mathbb{C}[^{\lambda}{\lambda}_1, ^{\lambda}{\lambda}_2, ^{\lambda}{\lambda}_3]$. This concludes the proof. □

### 3.2 The reference matrix

Following our choice of initialization and the previous results presented in Propositions 1 and 2, we consider a set of $p$ directions $\{d_i\}_{1 \leq i \leq p}$ defined by two angles $(\theta_l, \varphi_l)$ as follows:

\[
d_l = \begin{bmatrix} \sin \theta_l \sin \varphi_l \\ \sin \theta_l \cos \varphi_l \\ \cos \theta_l \end{bmatrix}.
\]

To describe the natural choice of reference case, we then define - for a common value $s \in \mathbb{C}$ and the matrices $P$ and $D$ from Hypothesis 1 - the functions:

\[
\chi_l : x \mapsto \exp sP^{-1/2}d_l \cdot (x - x_C),
\]
as well as the associated matrix in $\mathbb{C}^{(n+1)(n+2)(n+3)/6 \times p}$:

$$E_{n,p}^{n,p} = T_{\chi_1}[i].$$

Each entry $(N(i), l)$ being a multiple of $(\sin \varphi_1)^{i_1} (\cos \varphi_1)^{i_2} (\sin \theta_1)^{i_1+i_2} (\cos \theta_1)^{i_3}$, hence we define the associated matrix in $\mathbb{C}^{(n+1)(n+2)(n+3)/6 \times p}$:

$$R_{N(i), l} = \frac{(\sin \varphi_1)^{i_1} (\cos \varphi_1)^{i_2} (\sin \theta_1)^{i_1+i_2} (\cos \theta_1)^{i_3}}{i!}.$$

and show how they are related in the following result.

**Lemma 3.** Consider any set of $p$ directions $\{d_l\}_{1 \leq l \leq p}$ as well as the matrices $\mathcal{P}$ and $\mathcal{D}$ from Hypothesis [4] together with the associated $(n+1)(n+2)(n+3)/6 \times p$ complex matrices $E^{n,p}$ and $R^{n,p}$. There exists a block diagonal matrix $D^n \in \mathbb{C}^{(n+1)(n+2)(n+3)/6 \times (n+1)(n+2)(n+3)/6}$ such that $E^{n,p} = D^n R^{n,p}$ and $R^{n,p} = D^n E^{n,p}$, independently of their number $p$ of columns.

**Proof.** The entries of the reference matrix $E^{n,p}$ are:

$$T_{\chi_1}[i] = \frac{1}{i!} \left(\left(\mathcal{P} \mathcal{D}^{-1/2} d_l\right)_{j_1}^{i_1} \left(\mathcal{P} \mathcal{D}^{-1/2} d_l\right)_{j_2}^{i_2} \left(\mathcal{P} \mathcal{D}^{-1/2} d_l\right)_{j_3}^{i_3}\right),$$

and we consider row blocks corresponding to increasing values of $|i|$: for $m$ from $0$ to $n$ we denote by $E^{n,p}_{(m)}$ and $R^{n,p}_{(m)}$ the $(m+1)(m+2)/2 \times p$ blocks of rows corresponding to all $i$ such that $|i| = m$, that is

$$E^{n,p}_{(m)} = (E^{n,p})_{N_m(i)}, \quad R^{n,p}_{(m)} = (R^{n,p})_{N_m(i)}.$$

As a reminder, $s \in \mathbb{C}$ is a constant, while $\mathcal{P}$ and $\mathcal{D}$ depend only on the value of the PDE coefficients $c$ evaluated at $x_C$, hence the entries of the $3 \times 3$ matrix $s \mathcal{P} \mathcal{D}^{-1/2}$ are independent of $l$; moreover the matrix $s \mathcal{P} \mathcal{D}^{-1/2}$ is non-singular under Hypothesis [4]. Thus, according to Lemma [4] below for $A := s \mathcal{P} \mathcal{D}^{-1/2}$, for all $m$ from $0$ to $n$ there exist an $(m+1)(m+2)/2 \times (m+1)(m+2)/2$ matrix $C^{(m)}$, defined entry-wise by 

$$(C^{(m)})_{N_m(i)N_m(j)} = c_{ij},$$

such that $E^{n,p}_{(m)} = C^{(m)} R^{n,p}_{(m)}$ and $R^{n,p}_{(m)} = C^{(m)} E^{n,p}_{(m)}$.

Defining the block diagonal matrix $D^n := (C^{(0)}, C^{(1)}, \ldots, C^{(n)})$, we then obtain the desired property: $E^{n,p} = D^n R^{n,p}$ and $R^{n,p} = D^n E^{n,p}$. \hfill \Box

**Lemma 4.** Let $A \in \mathbb{C}^{3 \times 3}$ be non-singular. Then, for any vector $Y \in \mathbb{C}^3$, any product of powers of the entries of $AY$ with a total power $m \in \mathbb{N}$ can be written as a linear combination depending only on $A$ but independent of $Y$ - of products of powers of the entries of $Y$ each one of the products having a total power equal to $m$. Mathematically speaking:

$$\forall i \in (\mathbb{N}_0)^3, \exists \{c_{ij} \in \mathbb{C}, j \in (\mathbb{N}_0)^3, |j| = |i|\} \text{ such that } \forall Y \in \mathbb{C}^3, \prod_{k=1}^3 (\text{(AY)k})^{i_k} = \sum_{|j|=|i|} c_{ij} \prod_{l=1}^3 (Y_l)^{j_l}. \quad (24)$$

Moreover:

$$\forall X \in \mathbb{C}^3, \prod_{k=1}^3 (X_k)^{i_k} = \sum_{|j|=|i|} c_{ij} \prod_{l=1}^3 ((A^{-1} X)_l)^{j_l}. \quad (25)$$

**Remark 5.** The result still holds for $n \in \mathbb{N}$ and $A \in \mathbb{C}^{n \times n}$, the proof is more tedious as it requires the introduction of more indices. In this article we only use the $n = 3$ case hence we do not prove the more general case.

**Proof.** Since, for $k \in \{1, 2, 3\}$ and any $3 \times 3$ matrix $A$, we have:

$$(\text{(AY)k})^{i_k} = \left(\sum_{l=1}^3 A_{kl} Y_l\right)^{i_k} = \sum_{|j|=i_k} \frac{(i_k)!}{j!} \prod_{l=1}^3 (A_{kl} Y_l)^{j_l} = \sum_{|j|=i_k} \frac{(i_k)!}{j!} \prod_{l=1}^3 (A_{kl})^{j_l} \prod_{l=1}^3 (Y_l)^{j_l},$$

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then we get:
\[
\prod_{k=1}^{3} ((AY)_k)^{i_k} = \sum_{|j|=1}^{3} \sum_{|j'|=1}^{3} \sum_{|j''|=1}^{3} \frac{i!}{j!(j')!(j'')!} \left( \prod_{l=1}^{3} (A_{1l})^{j_l} (A_{2l})^{j'_l} (A_{3l})^{j''_l} \right) \prod_{l=1}^{3} (Y_l)^{j_l+j'_l+j''_l}.
\]

This concludes the proof of (24), as \( \sum_{l=1}^{3} (j_l + j'_l + j''_l) = |j| + |j'| + |j''| = i_1 + i_2 + i_3 = |i| \).

Moreover, if \( A \) is non-singular, then, for any \( X \in \mathbb{C}^3 \), (24) applied to \( Y = A^{-1}X \) shows (25).

As a direct consequence we have the following results.

**Corollary 1.** Given \((n, p) \in \mathbb{N}^2\) and any choice of \( p \) directions \( \{d_l \in S^2\}_{1 \leq l \leq p} \), the rank of \( E^{n,p} \) is equal to the rank of \( R^{n,p} \).

**Corollary 2.** Similarly, any pair of sub-matrices of \( E^{n,p} \) and \( R^{n,p} \) corresponding to removing the same sets of all rows \( i \) with \( |i| = m \) for a given \( m \) - in particular removing all rows \( i \) with \( |i| > 1 \) - have the same rank.

The next step is to study the rank of these matrices, and the following step will be to relate it to the rank of the quasi-Trefftz matrices \( A, P \) and \( Q \).

### 3.3 Properties of the reference matrix

We are interested here in the rank of the reference matrix, \( R^{n,p} \), or equivalently the rank of the exponential matrix \( E^{n,p} \) according to Corollary [1] as well as the rank of some of their useful sub-matrices. In particular the rank’s value depends on the number of columns \( p \), and we will see that:

- independently of the number of columns \( p \), the rank is at most \((n + 1)^2\),
- while there exist sets of \( p = (n + 1)^2 \) directions that guarantee the rank of the corresponding matrix to be maximal, that is \((n + 1)^2\).

To study this reference matrix, we first remark that its entries are a set of functions, on each row, evaluated at a set of points, on each column. The following result provides the maximum possible rank of such matrices depending on the dimension of the space generated by the function set.

**Lemma 5.** Consider a set \( \mathcal{D} \) of \( N_f \) complex-valued functions defined on a domain \( \Omega \) (in any dimension), denoted \( \mathcal{D} \), while the dimension of span \( \mathcal{D} \) is \( N_d < N_f \). We consider any \( N_f \times N_p \) matrix \( \mathcal{D} \) defined element wise by evaluating the elements of the function space \( \mathcal{D} \) at a set of \( N_p \) points \( \{\Theta_l \in \Omega\}_{1 \leq l \leq N_p} \), namely:

\[
\mathcal{D}_{kl} = d_k(\Theta_l).
\]

Then the rank of \( \mathcal{D} \) is at most equal to \( N_d \).

Moreover, if \( B \) is any generating set of span \( \mathcal{D} \), then the corresponding \( N_b \times N_p \) matrix \( B \), namely:

\[
B_{kl} = y_k(\Theta_l),
\]

has the same rank as \( \mathcal{D} \).

---

1This argument was previously presented in our roadmap paper for a particular case defined by the function space \( \mathcal{T}_n = \{\theta \mapsto \cos^k \theta \sin^{K-k} \theta/(k!(K-k)!), 0 \leq k \leq K \leq n\} \), containing \#\(\mathcal{T}_n = (n + 1)(n + 2)/2 \) functions and spanning a space of dimension \( \text{dim} \text{span}\mathcal{T}_n = 2n + 1 \).
Proof. Because of the number of elements in \( D \) and the dimension of its span, there exists a matrix \( C \in \mathbb{C}^{(N_f-N_d) \times N_f} \), of rank \( N_f-N_d \) such that
\[
\forall k' \in \mathbb{N}, k' \leq N_f-N_d, \sum_{k=1}^{N_f} C_{k'k} d_k = 0.
\]
In particular, independently of the number \( N_p \) of columns of \( D \), this yields:
\[
CD = 0_{(N_f-N_d) \times N_p}.
\]
Hence the \( N_p \) columns of \( D \) belong to the kernel of \( C \), which is of dimension \( N_d \) according to the rank-nullity theorem. So indeed the rank of \( D \) is at most equal to \( N_d \).

Moreover, consider a set \( \tilde{D} \subset D \), being a generating set for \( \text{span } D \), and the submatrix of \( D \), denoted \( \tilde{D} \) and obtained by keeping only the rows corresponding to each \( d_k \in D \). Since the space generated by the rows of \( D \) is the same as the space generated by the rows of \( \tilde{D}, D \) and \( \tilde{D} \) have the same rank. Similarly, consider \( B = \{y_k, 1 \leq k \leq N_b\} \) any generating set of \( \text{span } D \), then consider the corresponding matrix \( B \). Each of its rows can be written as a linear combination of the rows of \( D \), since \( \tilde{D} \) is a generating set of \( \text{span } D \), while each row of \( \tilde{D} \) can be written as a linear combination of the rows of \( B \), since \( B \) is also a generating set of \( \text{span } D \). This proves the second claim. \( \square \)

To address the particular case of the matrix \( R \), we then define the following functions and function space:
\[
\forall i \in (N_0)^3, f_i(\theta, \varphi) = (\sin \varphi)^{i_1}(\cos \varphi)^{i_2}(\sin \theta)^{i_1+i_2}(\cos \theta)^{i_3}/i!, \text{ and } F_n := \{f_i, i \in (N_0)^3, |i| \leq n\},
\]
\[
\tilde{F}_n := \{f_i, i \in (N_0)^3, |i| \leq n, i_1 \in \{0, 1\}\}.
\]
The space \( F_n \) contains \((n+1)(n+2)(n+3)/6\) elements, let’s now identify the dimension of \( \text{Span}\tilde{F}_n \). We will make use of the following functions and function spaces:
\[
Z_l^m(\theta, \varphi) = e^{im\varphi}(\sin \theta)^{|m|}(\cos \theta)^{-|m|} \text{ and } G_n := \{Z_l^m, 0 \leq l \leq n, -l \leq m \leq l\},
\]
and for the spherical harmonics with \( C_l^m = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \) and the Legendre polynomials \( P_l^m \) (see appendix B):
\[
Y_l^m(\theta, \varphi) := C_l^m P_l^m(\cos \theta) e^{im\varphi} \text{ and } H_n := \{Y_l^m, 0 \leq l \leq n, -l \leq m \leq l\}.
\]

Lemma 6. Given \( n \in \mathbb{N} \), the spaces of trigonometric functions and spherical harmonics are such that:
- \( \text{Span}\tilde{F}_n = \text{Span}\mathcal{F}_n = \text{Span}\mathcal{G}_n = \text{Span}\mathcal{H}_n \),
- they are all of dimension \((n+1)^2\).

Proof. Step 1. One clearly sees that \( \mathcal{F}_n \subset \mathcal{F}_n \), we show that every element of \( \mathcal{F}_n \) belongs to \( \text{Span}\mathcal{F}_n \).

Considering any function \( f_i \) in \( \mathcal{F}_n \), according to \( i_1 \) being even or odd, we will treat the two cases as follows.

If \( i_1 \) is even, since \((\sin \varphi)^{i_1} = (1-\cos^2 \varphi)^{i_1/2} \), then we have:
\[
f_i(\theta, \varphi) = \sum_{k_\varphi=0}^{i_1/2} \binom{i_1/2}{k_\varphi} (-1)^{k_\varphi} (\cos \varphi)^{2k_\varphi} (\sin \theta)^{i_1+i_2}(\cos \theta)^{i_3}/i!.
\]
and since \((\sin \theta)^{i_1+i_2} = (\sin \theta)^{2i_1+i_2}(1-\cos^2 \varphi)^{i_1/2-k_\varphi} \), we can write:
\[
f_i(\theta, \varphi) = \sum_{k_{\varphi}=0}^{i_1/2} \sum_{k_\theta=0}^{i_1/2-k_\varphi} \binom{i_1/2}{k_\varphi} \binom{i_1/2-k_\varphi}{k_\theta} (-1)^{k_\varphi+k_\theta} \sin^0 \theta (\cos \varphi)^{2k_\varphi+i_2}(\sin \theta)^{i_1+i_2}(\cos \theta)^{2k_\theta+i_3}/i!.
\]
We then easily see that $0 + (2k_\varphi + i_2) = 2k_\varphi + i_2$ while $(2k_\varphi + i_2) + (2k_\theta + i_3) \leq 2k_\varphi + i_2 + i_1 - 2k_\varphi + i_3 = |i|$, hence in particular $f_i \in \text{Span} \mathcal{F}_n$.

If $i_1$ is odd, since $(\sin \varphi)^{i_1} = \sin \varphi (1 - \cos^2 \varphi)^{(i_1-1)/2}$, then we have:

$$f_i(\theta, \varphi) = \sum_{k_\varphi=0}^{(i_1-1)/2} \left( \frac{(i_1 - 1)/2}{k_\varphi} \right) (-1)^{k_\varphi} \sin \varphi (\cos \varphi)^{2k_\varphi+i_2} (\sin \theta)^{i_1+i_2}(\cos \theta)^{i_3}/i!,$$

and since $(\sin \theta)^{i_1+i_2} = (\sin \theta)^{2k_\varphi+1+i_2} (1 - \cos^2 \theta)^{(i_1-1)/2-k_\varphi}$, we can write:

$$f_i(\theta, \varphi) = \sum_{k_\varphi=0}^{i_1-1} \sum_{k_\theta=0}^{i_2-1} \left( \frac{1}{k_\varphi} \left( \frac{i_1 - 1}{2k_\varphi} - \frac{1}{2k_\theta} \right) \right) (-1)^{k_\varphi+k_\theta} \sin \varphi (\cos \varphi)^{2k_\varphi+i_2} (\sin \theta)^{2k_\varphi+1+i_2}(\cos \theta)^{2k_\theta+i_3}/i!.$$

We then easily verify that $1 + (2k_\varphi + i_2) = 2k_\varphi + 1 + i_2$ while $(2k_\varphi + 1 + i_2) + (2k_\theta + i_3) \leq 2k_\varphi + 1 + i_2 + i_1 - 2k_\varphi + i_3 = |i|$, hence again $f_i \in \text{Span} \mathcal{F}_n$.

This proves that $\text{Span} \mathcal{F}_n = \text{Span} \mathcal{F}_n$.

**Step 2.** Let’s start by considering any element $f_i$ of $\mathcal{F}_n$ to show that it belongs to $\text{Span} \mathcal{G}_n$. For all $i \in \mathbb{N}_0^3$ such that $|i| \leq n$, writing $\cos \varphi, \sin \varphi$ under their exponential form, and expanding their powers according to the binomial formula, we have:

$$f_i(\theta, \varphi) = \frac{1}{i!(2i_1)^{2i_2}}(\sin \varphi)^{i_1+i_2} \left( \sum_{j_1=0}^{i_1} \sum_{j_2=0}^{i_2} (-1)^{j_1} \binom{i_1}{j_1} \binom{i_2}{j_2} \exp (i(i_1 - 2j_1 + i_2 - 2j_2)\varphi) \right) (\cos \theta)^{i_3}.$$

In order to write each $(\sin \theta)^{i_1+i_2} \exp (i(i_1 - 2j_1 + i_2 - 2j_2)\varphi)(\cos \theta)^{i_3}$ term in this sum as a linear combination of $Z_l^m$, the power of $\sin \theta$ must be the absolute value of the power of $\exp i\varphi$. Therefore, defining $M_{i_1,j_1,j_2} := \min(i_1 - j_1 + i_2 - j_2, j_1 + j_2)$, we can write $i_1 + i_2$ independently of the sign of $i_1 - 2j_1 + i_2 - 2j_2$ as:

$$i_1 + i_2 = |i_1 - 2j_1 + i_2 - 2j_2| + 2M_{i_1,j_1,j_2}.$$

This leads to

$$(\sin \theta)^{i_1+i_2} \exp (i(i_1 - 2j_1 + i_2 - 2j_2)\varphi)(\cos \theta)^{i_3} = (\sin \theta)^{|i_1-2j_1+i_2-2j_2|}(1 - \cos^2 \theta)^{M_{i_1,j_1,j_2}} \exp (i(i_1 - 2j_1 + i_2 - 2j_2)\varphi)(\cos \theta)^{i_3}$$

$$= \sum_{j_3=0}^{M_{i_1,j_1,j_2}} \binom{M_{i_1,j_1,j_2}}{j_3} (-1)^{j_3} (\sin \theta)^{|i_1-2j_1+i_2-2j_2|}(\cos \theta)^{2j_3+i_3} \exp (i(i_1 - 2j_1 + i_2 - 2j_2)\varphi),$$

so

$$f_i(\theta, \varphi) = \frac{1}{i!(2i_1)^{2i_2}} \sum_{j_1=0}^{i_1} \sum_{j_2=0}^{i_2} \sum_{j_3=0}^{M_{i_1,j_1,j_2}} (-1)^{j_1} \binom{i_1}{j_1} \binom{i_2}{j_2} \sum_{j_3=0}^{M_{i_1,j_1,j_2}} \binom{M_{i_1,j_1,j_2}}{j_3} (-1)^{j_3} Z_{|i_1-2j_1+i_2-2j_2|+2j_3+i_3}^{i_1-2j_1+i_2-2j_2}(\theta, \varphi).$$

To verify that these $Z_l^m$ belong to the space $\text{Span} \mathcal{G}_n$, we must make sure that their indices satisfy $0 \leq l \leq n$ and $|m| \leq l$. In fact:

- if $i_1 - 2j_1 + i_2 - 2j_2 \geq 0$ then
  $$j_3 \leq j_1 + j_2 \Rightarrow i_1 - 2j_1 + i_2 - 2j_2 + 2j_3 + i_3 \leq i_1 + i_2 + i_3,$$
  $$i_1 - 2j_1 + i_2 - 2j_2 \geq 0 \Rightarrow i_1 - 2j_1 + i_2 - 2j_2 + 2j_3 + i_3 \geq 0,$$
  $$i_1 - 2j_1 + i_2 - 2j_2 = |i_1 - 2j_1 + i_2 - 2j_2| \Rightarrow |i_1 - 2j_1 + i_2 - 2j_2| \leq i_1 - 2j_1 + i_2 - 2j_2 + 2j_3 + i_3.$$

- if $i_1 - 2j_1 + i_2 - 2j_2 < 0$ then
  $$j_3 \leq i_1 - j_1 + i_2 - j_2 \Rightarrow 2j_1 - i_1 + 2j_2 - i_2 + 2j_3 + i_3 \leq i_1 + i_2,$$
  $$2j_1 - i_1 + 2j_2 - i_2 \geq 0 \Rightarrow 2j_1 - i_1 + 2j_2 - i_2 + 2j_3 + i_3 \geq 0,$$
  $$2j_1 - i_1 + 2j_2 - i_2 = |i_1 - 2j_1 + i_2 - 2j_2| \Rightarrow |2j_1 - i_1 + 2j_2 - i_2| \leq 2j_1 - i_1 + 2j_2 - i_2 + 2j_3 + i_3.$$
To summarize, since \( i_1 + i_2 + i_3 = |i| \), the indices of each \( Z_{i_1-2j_1+i_2-2j_2+i_3-2j_3} \) are such that:

\[
\left\{ \begin{align*}
|i_1 - 2j_1 + i_2 - 2j_2| + 2j_3 + i_3 & \leq |i|, \\
|i_1 - 2j_1 + i_2 - 2j_2| + 2j_3 + i_3 & \geq 0, \\
|i_1 - 2j_1 + i_2 - 2j_2| & \leq |i_1 - 2j_1 + i_2 - 2j_2| + 2j_3 + i_3.
\end{align*} \right.
\]

Hence, for \( |i| \leq n \), \( f_i \) can indeed be written as a linear combination of \( Z_{|i|}^l \) with \( 0 \leq l \leq n \) and \( |m| \leq l \). In other words, each element of \( \mathcal{F}_n \) can be written as a linear combination of \( f_i \)s. In fact, expanding \( e^{i m \varphi} \) via the binomial formula we immediately see that for all \((l, m) \in \mathbb{Z}^2\) such that \( 0 \leq l \leq n \) and \(-l \leq m \leq l\) we have:

\[
Z_{l,m}^\pm (\theta, \varphi) = \sum_{m' = 0}^{\lfloor |m| \rfloor} (|m| - m')! (\cos \varphi)^{m'} (\pm i \sin \varphi)^{|m| - m'} (\sin \theta)^{|m|} (\cos \theta)^{l - |m|},
\]
or equivalently

\[
Z_{l,m}^\pm (\theta, \varphi) = \sum_{m' = 0}^{\lfloor |m| \rfloor} (\pm i)^{|m| - m'} (|m|)! (l - |m|)! f_{(|m| - m', m', l - |m|)}, \text{ where } \left( |m| - m', m', l - |m| \right) = l \leq n,
\]
hence each element of \( \mathcal{G}_n \) belongs to \( \text{Span}{\mathcal{F}_n} \).

As a consequence, \( \text{Span}{\mathcal{G}_n} = \text{Span}{\mathcal{F}_n} \).

**Step 3.** Any function in \( \mathcal{H}_n \) can be written as

if \( m \geq 0 \), \( Y_l^m(\theta, \phi) = C_l^m \frac{(-1)^m}{2^l!} (\sin \theta)^m e^{im\phi} \sum_{l' = \lfloor l/2 \rfloor}^l \left( \begin{array}{c} l \\ l' \end{array} \right) (-1)^{l-l'} \frac{(2l')!}{(2l' - l - m)!} (\cos \theta)^{2l' - l - m} Z_{2l'-l}^m \)

and

if \( m < 0 \), \( Y_l^m(\theta, \phi) = C_l^m \frac{(l - |m|)!}{(l + |m|)!} \frac{1}{2^l!} (\sin \theta)^m e^{im\phi} \sum_{l' = \lfloor l/2 \rfloor}^l \left( \begin{array}{c} l \\ l' \end{array} \right) (-1)^{l-l'} \frac{(2l')!}{(2l' - l - m)!} (\cos \theta)^{2l' - l - |m|} Z_{2l'-l}^m \)

hence each element of \( \mathcal{H}_n \) belongs to \( \text{Span}{\mathcal{G}_n} \). So \( \text{Span}{\mathcal{H}_n} \subset \text{Span}{\mathcal{G}_n} \).

Moreover, by property of the spherical harmonics, these are linearly independent, therefore

\[
\dim \mathcal{H}_n = (n + 1)^2.
\]

We have then shown that

\[
(n + 1)^2 \leq \dim \text{Span}{\mathcal{G}_n}.
\]

But the space \( \mathcal{G}_n \) has \((n + 1)^2\) elements, so \( \dim \text{Span}{\mathcal{G}_n} = (n + 1)^2 \).

**Conclusion** The result follows trivially from combining the previous steps.

As direct consequences of Lemmas 5 and 6 as well as Corollaries 1 and 2 we get the following.

**Corollary 3.** Given \((n, p) \in \mathbb{N}^2\), for any choice of \( p \) directions \( \{d_i\}_{1 \leq i \leq p} \), the rank of \( \mathbb{E}^{n,p} \), and hence the rank of \( \mathbb{R}^{n,p} \), cannot be larger than \((n + 1)^2\). Moreover the submatrices \( \mathbb{E}^{n,p}_{k,l} \) and \( \mathbb{R}^{n,p}_{k,l} \) have the same rank as \( \mathbb{R}^{n,p} \) as well.

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The next natural question is that of existence of a set of \((n+1)^2\) directions \(\{(\theta_i, \varphi_i) \in \mathbb{R}^2\}_{1 \leq i \leq (n+1)^2}\) such that the corresponding matrices are of rank \((n+1)^2\). Hence it is natural to now fix \(p = (n+1)^2\), denoting hereafter the corresponding matrices \(E^{[n]}\) and \(R^{[n]}\). If such a set of directions exists, then increasing the value of \(p\) will not increase the rank according to Corollary 3.

**Theorem 1.** Given \(n \in \mathbb{N}\), let \(p = (n+1)^2\) directions on \(\mathbb{S}^2\) be chosen as:

\[
d_{l,m} = (\sin \theta_l \cos \varphi_{lm}, \sin \theta_l \sin \varphi_{lm}, \cos \theta_l)
\]

for all \(l\) from 0 to \(n\) with \(|m| \leq l\), where the \(n+1\) colatitude angles \(\{\theta_i\}_{0 \leq i \leq n} \subset (0, \pi)\) are all different from each other, and the azimuths \(\{\varphi_{lm}\}_{0 \leq l \leq n, |m| \leq l} \subset [0, 2\pi)\) satisfy \(\varphi_{lm} \neq \varphi_{lm'}\) for every \(m \neq m'\). Then the two \(\frac{(n+1)(n+2)(n+3)}{6} \times (n+1)^2\) matrices \(R^{[n]}\) and \(E^{[n]}\) are of rank \((n+1)^2\).

Moreover, their square sub-matrices of \(R^{[n]}\) and \(E^{[n]}\) corresponding to removing the rows \(i\) such that \(i_1 > 1\), denoted respectively \(R^{[n]}\) and \(E^{[n]}\), are also of rank \((n+1)^2\).

Here again, properties of spherical harmonics will be at the center of the proof.

**Proof.** Since \(H_n\) is a generating set for \(Span F_n\), then according to Lemma 5, the rank of \(R^{[n]}\) is that of the \((n+1)^2 \times (n+1)^2\) matrix \(S_n\) defined element wise by evaluating the elements of the function space \(H_n\). As stated in Lemmas 3.4.1 and 3.4.2 from [30], this matrix \(S_n\) is invertible. As a conclusion, \(R^{[n]}\) is indeed of rank \((n+1)^2\). As a direct consequence of Corollary 1, \(E^{[n]}\) is also of rank \((n+1)^2\).

Since \(F_n\) is a generating set for \(Span F_n\) from Lemma 6, applying the second statement from Lemma 5 then proves the second statement. \(\square\)

**Remark 6.** In terms of directions, the result is actually true for almost any set of points \(\{(\theta_i, \varphi_i) \in (0, \pi) \times [0, 2\pi)\}_{0 \leq i \leq n, |m| \leq l}\) as Lemma 3.4.1 from [30] states that the rank of the matrix \(S_n\) is \((n+1)^2\) for a dense open set of \((\mathbb{S}^2)^p\).

### 3.4 Relating quasi-Trefftz and reference matrices

We are now interested in the rank of the quasi-Trefftz matrices, namely the \((n+1)(n+2)(n+3)/6 \times p\) matrices \(A, P\) and \(Q\). In order to leverage the properties of the reference matrix to prove properties of these quasi-Trefftz matrices, the missing link is then to understand their relation to the reference matrix.

Because of their polynomial component, either in the phase, the amplitude, or the function itself, quasi-Trefftz functions have derivatives that share a common structure when evaluated at \(x_C\) as long as their order is not higher than \(q + 1\). Even though higher order derivatives could also be studied, they would not share this common structure. Hence we will start by studying the common properties of such derivatives of quasi-Trefftz functions. Under the assumption that \(q \geq n-1\), the entries in the quasi-Trefftz matrices are precisely such derivatives evaluated at \(x_C\). This will then allow us to establish a relation between the reference matrix and each of the quasi-Trefftz matrices.

Noticeably, neither the number of quasi-Trefftz functions chosen to construct each matrix, denoted \(p\), nor the set of directions in the initialization come into play in this procedure: we establish relations between matrices independently of both. However, proving that the quasi-Trefftz functions can be constructed to guarantee that the corresponding quasi-Trefftz matrices have maximal rank will rely on an appropriate choices for \(p\) and the set of directions.

#### 3.4.1 The GPW case

To address the two GPW cases, it is natural to start from expressing the derivatives of GPW functions in terms of the three non-zero free parameters in the initialization, leveraging Propositions 1 and 2.
Proposition 3. Given $q \in \mathbb{N}$ and a point $x_C \in \mathbb{R}^3$, a set of complex-valued functions $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ is assumed to satisfy Hypothesis $\mathbb{H}$.

Consider any amplitude-based GPW associated to partial differential operator $\mathcal{L}_c$, $J(x) := Q(x-x_C)\exp\Lambda \cdot (x-x_C)$ with $Q := \sum_{\mu \in \mathbb{N}_0^3, |\mu| \leq q+1} \mu_i X^i$, constructed via Algorithms 1 and 2 with the initialization introduced in Section 2.7 for $s \in \mathbb{C}^*$ and a unit vector $d \in \mathbb{S}^2$. Then, for all $j \in (\mathbb{N}_0)^3$ such that $|j| \leq q + 1$, the difference $\partial^j_x J(x_C)/j! - (\Lambda_1)^j_1 (\Lambda_2)^j_2 (\Lambda_3)^j_3 / j!$ can be expressed as a polynomial in $\mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3]$, with degree smaller than $|j|$ and coefficients depending on $s$ yet independent of $d$.

Proof. Since $J(x) := Q(x-x_C)\exp\Lambda \cdot (x-x_C)$, we can express $\partial^j_x J$ thanks to Leibniz’s rule as:

$$\forall x \in \mathbb{R}^3, \partial^j_x J(x) = \sum_{j \leq j} \left(\frac{j}{j}\right) \Lambda^j_\tilde{j} \partial^j_x Q(x-x_C),$$

and therefore

$$\partial^j_x J(x_C) = \sum_{j \leq j} \frac{j!}{(j-j)!} \Lambda^j_\tilde{j} \mu^\tilde{j}.$$ 

Let’s consider the terms in this linear combination, starting from considering the possible degree of each individual term as a polynomial in $\mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3]$:

1. for $|\tilde{j}| = 0$, then $\Lambda^j_\tilde{j} \mu^\tilde{j} = (\Lambda_1)^j_1 (\Lambda_2)^j_2 (\Lambda_3)^j_3$ is a polynomial of degree $|j|$,

2. for $|\tilde{j}| = 1$, then $\Lambda^j_\tilde{j} \mu^\tilde{j} = 0$,

3. for $|\tilde{j}| > 1$, then $\Lambda^j_\tilde{j} \mu^\tilde{j}$ can be expressed as a polynomial of degree at most equal to $|j-j| + |\tilde{j}| - 1 < |j|$ according Proposition $\mathbb{H}$.

In the first case, the corresponding weight in the linear combination is precisely $j!/j! = 1$, while all other terms can be expressed as a polynomial in $\mathbb{C}[\Lambda_1, \Lambda_2, \Lambda_3]$ with total degree smaller than $|j|$. This concludes the proof.

These polynomials have coefficients independent of $d$ as a consequence of Proposition $\mathbb{H}$. $\square$

Proposition 4. Given $q \in \mathbb{N}$ and a point $x_C \in \mathbb{R}^3$, a set of complex-valued functions $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ is assumed to satisfy Hypothesis $\mathbb{H}$.

Consider any phase-based GPW associated to differential operator $\mathcal{L}_c$, $G(x) := \exp P(x-x_C)$ with $P := \sum_{i \in \mathbb{N}_0^3, |i| \leq q+1} \lambda_i X^i$, constructed via Algorithms 1 and 2 with the initialization introduced in Section 2.7 for $s \in \mathbb{C}^*$ and a unit vector $d \in \mathbb{S}^2$. Then, for all $j \in (\mathbb{N}_0)^3$ such that $|j| \leq q + 1$, the difference $\partial^j_x G(x_C)/j! - (\lambda_1)^j_1 (\lambda_2)^j_2 (\lambda_3)^j_3 / j!$ can be expressed as a polynomial in $\mathbb{C}[\lambda_1, \lambda_2, \lambda_3]$, with degree smaller than $|j|$ and coefficients depending on $s$ yet independent of $d$.

Proof. Since $G(x) = \exp P(x-x_C)$, we can express $\partial^j_x G$ thanks to Faa di Bruno’s formula (see Appendix $\mathbb{C}$) as:

$$\forall x \in \mathbb{R}^3, \partial^j_x G(x) = \sum_{1 \leq m \leq |j|} \exp(P(x-x_C)) \sum_{s=1}^{\frac{|j|}{s}} \sum_{l=1}^{\frac{|j|}{s}} \frac{j!}{s!} \prod_{m=1}^{s} \frac{1}{k_m!} \left(\frac{1}{l_m!} \partial^l_{x^m} P(x-x_C)\right)^{k_m},$$

where sets $p_s$ as well as indices $l_m$ and $k_m$ are as defined in Appendix $\mathbb{C}$ and therefore

$$\partial^j_x G(x_C) = \sum_{1 \leq m \leq |j|} \sum_{s=1}^{\frac{|j|}{s}} \sum_{l=1}^{\frac{|j|}{s}} \frac{j!}{s!} \prod_{m=1}^{s} \frac{1}{k_m!} \left(\lambda_{l_m}\right)^{k_m}.$$ 

Let’s consider the terms in this linear combination, starting from considering the possible degree of each individual $\lambda_{l_m}$ term as a polynomial in $\mathbb{C}[\lambda_1, \lambda_2, \lambda_3]$: 33
1. if \(|l_m| = 1\), then \(\lambda_m\) is a polynomial of degree 1,

2. if \(|l_m| > 1\), then \(\lambda_m\) can be expressed as a polynomial of degree \(\leq |l_m| - 1\) according to Proposition 2.

Thus each \(\prod_{m=1}^{s} (\lambda_{l_m})^{k_m}\) can be expressed as a polynomial in \(\mathbb{C}[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]\) with total degree at most equal to:

\[
\sum_{|l_m|=1} k_m + \sum_{|l_m|>1} k_m(|l_m| - 1).
\]

Each partition of \(j\) either does or does contain any \(l_m\) such that \(|l_m| \neq 1\). Accordingly, each \(\prod_{m=1}^{s} (\lambda_{l_m})^{k_m}\) falls into one of the two following categories, it can be expressed as a polynomial with total the degree:

1. either equal to \(\sum_{m=1}^{s} k_m = \tilde{m}\), when the partition contains only \(l_m\) such that \(|l_m| = 1\);
2. or smaller than \(\sum_{m=1}^{s} k_m = \tilde{m} \leq |j|\), when the partition contains at least one \(l_m\) such that \(|l_m| \neq 1\).

In the first case, each \(l_m\) belongs to \(\{e_1, e_2, e_3\}\), and, since the partition must satisfy \(\sum_{m=1}^{s} k_m l_m = j\), it corresponds to \(s = 3\) with \(j = j_1 e_1 + j_2 e_2 + j_3 e_3\). Hence \((\lambda_{e_1})^{j_1}(\lambda_{e_2})^{j_2}(\lambda_{e_3})^{j_3}\) is precisely of degree equal to \(|j|\), with a weight of \(\frac{1}{j_1 j_2 j_3} = 1\), whereas all other \(\prod_{m=1}^{s} (\lambda_{l_m})^{k_m}\) terms can be expressed as a polynomial in \(\mathbb{C}[\lambda_{e_1}, \lambda_{e_2}, \lambda_{e_3}]\) with total degree smaller than \(|j|\). This concludes the proof.

These polynomials have coefficients independent of \(d\) as a consequence of Proposition 2. \(\square\)

Since Propositions 3 and 4 state similar relations between the derivatives of GPW functions on the one hand and the three initialization parameters on the other hand, we can now prove the common property of both families of GPWs.

**Proposition 5.** Given \((n, p) \in \mathbb{N}^2\) and a point \(x_C \in \mathbb{R}^3\), a set of complex-valued functions \(c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}\) is assumed to satisfy Hypothesis 1.

Consider any sets of phase-based and amplitude-based GPWs associated to partial differential operator \(\mathcal{L}_c\), constructed via Algorithms 1 to 3, with \(q = \max(n - 1, 1)\) and the initialization introduced in Section 2.7 for \(s \in \mathbb{C}^*\) and any set of unit vectors \(\{d_l \in S^2, 1 \leq l \leq p\}\). Then there exist square lower triangular matrices \(L^n_A\) and \(L^n_P\), whose diagonal coefficients are equal to 1 and whose other non-zero coefficients depend only on (i) derivatives of the PDE coefficients \(c\) evaluated at \(x_C\) and (ii) the initialization parameter \(s\), such that

\[
A^{n,p} = L^n_A E^{n,p} \quad \text{and} \quad P^{n,p} = L^n_P E^{n,p}.
\]

As a result, we have:

\[
\text{rk}(A^{n,p}) = \text{rk}(E^{n,p}) \quad \text{and} \quad \text{rk}(P^{n,p}) = \text{rk}(E^{n,p}).
\]

**Proof.** This is a direct consequence of Propositions 3 and 4 and the choice of numbering for the matrix entries. Indeed:

- as a consequence of Propositions 3 and 4, for all \(j\) such that \(|j| \leq q\) there exist coefficients denoted \(l_{ij}^A\) and \(l_{ij}^P\) for \(i \in \mathbb{N}_0^3\) with \(|i| < |j|\) satisfying for any vector \(d\) and the corresponding amplitude- or phase-based GPW function, denoted respectively \(J\) or \(G\), for \(|j| > 0\):

\[
\partial^j_\xi J(x_C) = (\Lambda_1)^{j_1}(\Lambda_2)^{j_2}(\Lambda_3)^{j_3} + \sum_{|i|<|j|} l_{ij}^A (\Lambda_1)^{i_1}(\Lambda_2)^{i_2}(\Lambda_3)^{i_3}
\]

\[
\partial^j_\xi G(x_C) = (\lambda_{e_1})^{j_1}(\lambda_{e_2})^{j_2}(\lambda_{e_3})^{j_3} + \sum_{|i|<|j|} l_{ij}^P (\lambda_{e_1})^{i_1}(\lambda_{e_2})^{i_2}(\lambda_{e_3})^{i_3}
\]

while for \(|j| = 0\) both GPWs satisfy:

\[
J(x_C) = 1 \quad \text{and} \quad G(x_C) = 1;
\]

\(34\)
we can then define two square matrices of size \((n+1)(n+2)(n+3)/6\), \(L^n_A\) and \(L^p_P\), by:

\[
(L^n_A)_{N(j),N(i)} = \begin{cases} 
1 & \text{if } i = j, \\
\frac{1}{n!} a_{ij}^A & \text{if } |i| < |j|, \\
0 & \text{otherwise},
\end{cases}
\]

and similarly \((L^p_P)_{N(j),N(i)} = \begin{cases} 
1 & \text{if } i = j, \\
\frac{1}{p!} a_{ij}^P & \text{if } |i| < |j|, \\
0 & \text{otherwise},
\end{cases}\)

both lower triangular matrices since \(|i| < |j|\) implies that \(N(i) < N(j)\).

therefore, by definition of the matrices \(A^{n,p}\), \(P^{n,p}\) and \(R^{n,p}\), for \(j \in (\mathbb{N}_0)^3 \times \mathbb{N}\) with \(|j| \leq n\) and \(l \leq p\), we have the following relations:

\[
\begin{align*}
A^{n,p}_{N(j),l} &= \sum_{k=1}^{(n+1)(n+2)(n+3)} (L^n_A)_{N(j),k} R^{n,p}_{k,l} \\
P^{n,p}_{N(j),l} &= \sum_{k=1}^{(n+1)(n+2)(n+3)} (L^p_P)_{N(j),k} R^{n,p}_{k,l}
\end{align*}
\]

Fixing \(p = (n+1)^2\), we denote hereafter the corresponding \((n+1)(n+2)(n+3)/6 \times (n+1)^2\) matrices \(A^{[n]} := A^{n,(n+1)^2/2}\) and \(P^{[n]} := P^{n,(n+1)^2/2}\). As a direct consequence of Theorem 1 we then obtain the following result.

**Corollary 4.** Given \(n \in \mathbb{N}\) and a point \(x_C \in \mathbb{R}^3\), a set of complex-valued functions \(c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}\) is assumed to satisfy Hypothesis 2.

Let \(p = (n+1)^2\) directions on \(S^2\) be chosen as:

\[
d_{l,m} = (\sin \theta_l \cos \varphi_{lm}, \sin \theta_l \sin \varphi_{lm}, \cos \theta_l)
\]

for all \(l\) from 0 to \(n\) with \(|m| \leq l\), where the \(n+1\) colatitude angles \(\{\theta_l\}_{0 \leq l \leq n} \subset (0, \pi)\) are all different from each other, and the azimuths \(\{\varphi_{lm}\}_{0 \leq l \leq n, |m| \leq l} \subset [0, 2\pi)\) satisfy \(\varphi_{lm} \neq \varphi_{lm'}\) for every \(m \neq m'\). Consider any sets of phase-based and amplitude-based GPWs associated to partial differential operator \(L_c\) constructed via Algorithms 2 to 4, with \(q = \max(n-1, 1)\) the initialization introduced in Section 2.7 for \(s \in \mathbb{C}^*\) and directions \(\{d_{l,m}, 0 \leq l \leq n, |m| \leq l\}\). Then the corresponding matrices \(A^{[n]}\) and \(P^{[n]}\), of size \((n+1)(n+2)(n+3)/6 \times (n+1)^2\) are of rank \((n+1)^2\).

### 3.4.2 The polynomial case

To address the polynomial case, we consider again the corresponding Taylor expansion matrix, but in a different way that for the GPW case: thanks to the choice of initialization, only some of the rows of the matrix will be sufficient to study the desired rank properties.

**Proposition 6.** Given \(q \in \mathbb{N}\) and a point \(x_C \in \mathbb{R}^3\), a set of complex-valued functions \(c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}\) is assumed to satisfy Hypothesis 2.

Consider any polynomial quasi-Trefftz function associated to partial differential operator \(L_c\), \(H(x) := R(x - x_C)\) with \(R := \sum_{i \in \mathbb{N}_0^3, |i| \leq q+1} \nu_i X^i\), constructed via Algorithms 2 and 4, with the initialization introduced in Section 2.7 for \(s \in \mathbb{C}^*\) and a unit vector \(d\). Then, for all \(j \in (\mathbb{N}_0)^3\) such that \(|j| \leq q + 1\) and \(j_1 \in \{0, 1\}\) then \(\partial^2 H(x_C)/j! = (\nu_{e_1})^{j_1}(\nu_{e_2})^{j_2}(\nu_{e_3})^{j_3}\).

**Proof.** Since \(H(x) = R(x - x_C)\), we can express \(\partial^2 H\) directly as:

\[
\forall x \in \mathbb{R}^3, \partial^2 H(x) = \partial^2 R(x - x_C),
\]

and therefore

\[
\partial^2 H(x_C) = j! \nu_j.
\]

The result is then a direct consequence of the initialization (17).
We can then turn to the rank of $Q^{n,p}$, which will naturally be related to the rank of the sub-matrix of $E^{n,p}$ consisting of its rows corresponding to $i$ with $i_1 \in \{0,1\}$.

**Proposition 7.** Given $(n,p) \in \mathbb{N}^2$ and a point $x_C \in \mathbb{R}^3$, a set of complex-valued functions $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ is assumed to satisfy Hypothesis [1].

Consider any sets of polynomial quasi-Trefftz functions associated to partial differential operator $L_c$, constructed via Algorithms [1] and [4], with $q = \max(n - 1, 1)$ and the initialization introduced in Section 2.7 for $s \in \mathbb{C}^*$ and any set of directions $\{d_l \in \mathbb{S}^2, 1 \leq l \leq p\}$. Then

$$rk(E^{n,p}) \leq rk(Q^{n,p}).$$

**Proof.** If we denote by $R^{(n,p)}$ the sub-matrices of $R^{(n,p)}$ corresponding to removing the rows $i$ such that $i_1 > 1$, then, since $n \leq q + 1$, it becomes clear as a consequence of Proposition [6] that there exists a matrix $L_Q$ such that:

$$L_Q Q^{n,p} = R^{(n,p)}, \text{ so } rk(Q^{n,p}) \geq rk(R^{(n,p)}).$$

Moreover from Corollary [3] we have $rk(E^{n,p}) = rk(R^{(n,p)})$. This concludes the proof.

Fixing $p = (n + 1)^2$, we denote hereafter the corresponding matrix $Q^{[n]} := Q^{n,(n+1)^2}$. As a direct consequence of Theorem [1] we then obtain the following result.

**Corollary 5.** Given $n \in \mathbb{N}$ and a point $x_C \in \mathbb{R}^3$, a set of complex-valued functions $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ is assumed to satisfy Hypothesis [1].

Let $p = (n + 1)^2$ directions on $\mathbb{S}^2$ be chosen as:

$$\forall (l,m) \in (N_0)^2, l \leq n, |m| \leq l, d_{l,m} = (\sin \theta_l \cos \varphi_{lm}, \sin \theta_l \sin \varphi_{lm}, \cos \theta_l),$$

where the $n + 1$ colatitude angles $\{\theta_l\}_{0 \leq l \leq n} \subset (0, \pi)$ are all different from each other, and the azimuths $\{\varphi_{lm}\}_{0 \leq l \leq n, |m| \leq l} \subset [0, 2\pi)$ satisfy $\varphi_{lm} \neq \varphi_{lm'}$ for every $m \neq m'$. Consider any set of polynomial quasi-Trefftz functions associated to partial differential operator $L_c$, constructed via Algorithms [1] and [4], with $q = \max(n - 1, 1)$ and the initialization introduced in Section 2.7 for $s \in \mathbb{C}^*$ and directions $\{d_{l,m}, 0 \leq l \leq n, |m| \leq l\}$. Then the corresponding $(n+1)(n+2)(n+3)/6 \times (n + 1)^2$ matrix $Q^{[n]}$ is of rank $(n + 1)^2$.

### 3.5 Quasi-Trefftz bases Approximation properties

We finally want to show that the three spaces spanned by the quasi-Trefftz function sets introduced in Section 2 satisfy the desired approximation property [4], via matching of $u_a$’s Taylor expansion to that of $u$ as announced in [15].

**Theorem 2.** Given $n \in \mathbb{N}$ and a point $x_C \in \mathbb{R}^3$, a set of complex-valued functions $c = \{c_i, i \in \mathbb{N}_0^3, |i| \leq 2\}$ is assumed to satisfy Hypothesis [4].

Consider the three quasi-Trefftz spaces associated to partial differential operator $L_c$, defined as the spaces spanned by each of the three following sets:

- the set of amplitude-based GPWs, constructed via Algorithms [1] and [4];
- the set of phase-based GPWs, constructed via Algorithms [1] and [5];
- the set of polynomial functions, constructed via Algorithms [1] and [4];

each of them constructed with $q = \max(n - 1, 1)$ and the initialization introduced in Section 2.7 for $s \in \mathbb{C}^*$ and $p = (n + 1)^2$ directions on $\mathbb{S}^2$. If the set of directions is chosen as:

$$\forall (l,m) \in (N_0)^2, l \leq n, |m| \leq l, d_{l,m} = (\sin \theta_l \cos \varphi_{lm}, \sin \theta_l \sin \varphi_{lm}, \cos \theta_l),$$

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where the \( n + 1 \) colatitude angles \( \{ \theta_i \}_{0 \leq i \leq n} \subset (0, \pi) \) are all different from each other, and the azimuths \( \{ \varphi_{im} \}_{0 \leq i \leq n, |m| \leq i} \subset (0, 2\pi) \) satisfy \( \varphi_{im} \neq \varphi_{im'} \) for every \( m \neq m' \), then any of these three spaces, denoted \( \mathcal{V}^G_h \), satisfies the following approximation property:

\[
\forall u \in \mathcal{C}^{\max(2,n)}(\Omega) \text{ satisfying } \mathcal{L}_c u = 0, \exists u_a \in \mathcal{V}^G_h,
\exists C \in \mathbb{R} \text{ s.t. } \forall x \in \Omega, \begin{cases} |u(x) - u_a(x)| \leq C\|x - x_C\|^{n+1}, \\
\|\nabla u(x) - \nabla u_a(x)\| \leq C\|x - x_C\|^n. \end{cases}
\]  

(26)

The constant \( C \) here depends on the domain \( \Omega \), on the desired order \( n \), on the PDE solution \( u \) to be approximated, as well as on the PDE coefficients \( c \).

It is to be noted that this actually shows a convergence in the \( H^1 \) norm:

\[
\forall u \text{ satisfying } \mathcal{L} u = 0, \exists u_a \in \mathcal{V}, \exists C \in \mathbb{R}, \text{ s.t. } \|u - u_a\|_{H^1(B(x_C,h))} \leq Ch^n.
\]  

(27)

**Proof.** It is sufficient to prove that, if \( M^{[n]} \) is any of the three \((n+1)(n+2)(n+3)/6 \times (n+1)^2)\) quasi-Trefftz matrices, namely \( A^{[n]} \), \( P^{[b]} \) or \( Q^{[n]} \), then the linear system defined by:

\[
M^{[n]} \chi = F_n
\]

has a solution for any \( F_n \) in the vector space \( \mathbb{F}_{n,\mathcal{L}_c} \) defined as:

\[
\mathbb{F}_{n,\mathcal{L}_c} := \left\{ F \in \mathbb{C}^{(n+1)(n+2)(n+3)/6}, \exists v \in \mathcal{C}^{\max(2,n)}(\Omega) \text{ s.t. } \mathcal{L}_c v = 0 \text{ and } \forall i \in (N_0)^3, |i| \leq n, \ F_N(i) = \partial_i^j v(x_C)/i! \right\}.
\]

We first define a similar vector space by relaxing the Trefftz condition \( \mathcal{L}_c v = 0 \) into a quasi-Trefftz condition:

\[
\mathbb{K}_{n,\mathcal{L}_c} := \left\{ K \in \mathbb{C}^{(n+1)(n+2)(n+3)/6}, \exists v \in \mathcal{C}^{\max(2,n)}(\Omega) \text{ satisfying } \mathcal{L}_c v(x) = O(\|x - x_C\|^{n-1}) \text{ s.t. } \forall i \in (N_0)^3, |i| \leq n, \ K_N(i) = \partial_i^j v(x_C)/i! \right\}.
\]

It is then clear that \( \mathbb{F}_{n,\mathcal{L}_c} \subset \mathbb{K}_{n,\mathcal{L}_c} \), but also that the range of \( M^{[n]} \) is also included in \( \mathbb{K}_{n,\mathcal{L}_c} \).

Next we want to show that the dimension of \( \mathbb{K}_{n,\mathcal{L}_c} \) is \((n+1)^2\). For any function \( f \in \mathcal{C}^{\max(2,n)}(\Omega) \) satisfying \( \mathcal{L}_c f(x) = O(\|x - x_C\|^{n-1}) \), by Leibnitz rule we have:

\[
\forall i \in (N_0)^3, |i| \leq n, \sum_{|j| \leq 2} \sum_{1 \leq i} \binom{i}{j} \partial_{x}^{i-j} c_j \partial_x^j f(x_C) = 0.
\]

This shows that \( \mathbb{K}_{n,\mathcal{L}_c} \) is a subset of the kernel of an \((n-1)n(n+1)/6 \times (n+1)(n+2)(n+3)/6)\) matrix \( R \), with the following properties:

\[
\forall i \in (N_0)^3, |i| \leq n-2, \begin{cases} R_N(i)N(i+2e_1) = c_{2e_1}(x_C), \\
R_N(i)N(j) = 0 \text{ if } j > i + 2e_1.
\end{cases}
\]

Therefore, since \( c_{2e_1}(x_C) \neq 0 \) by Hypothesis \( \Box \) choosing a numbering scheme \( N \) such that if \( |i| = |j| \) then \( i < j \) implies \( N(i) \leq N(j) \) highlights the echelon structure of \( R \). As a result, the echelon structure of \( R \) guarantees that it has maximal rank, namely \((n-1)n(n+1)/6\), while its kernel is of dimension

\[
\frac{(n+1)(n+2)(n+3)}{6} - \frac{(n-1)n(n+1)}{6} = (n+1)^2.
\]

Hence \( \mathbb{K}_{n,\mathcal{L}_c} \) is a subset of a space of dimension \((n+1)^2\), but it also has a subset of the same dimension, namely the range of \( M^{[n]} \), so it is itself of dimension \((n+1)^2\).

This shows that the range of \( M^{[n]} \) and \( \mathbb{K}_{n,\mathcal{L}_c} \) are the same space, and therefore any \( F \in \mathbb{F}_{n,\mathcal{L}_c} \) belongs to the range of \( M^{[n]} \). So this conclude the proof of the approximation of the function values.

Precisely because this proof relies on matching the Taylor expansions of \( u \) and \( u_a \), the result of approximation of the gradient can be obtained directly by taking derivatives of this Taylor expansion matching identity.

\( \Box \)
4 Conclusion

Given a partial differential operator $L$ and a parameter $q \in \mathbb{N}$, a quasi-Trefftz function $f$ is a function satisfying the following local property in the neighborhood of a given point $x_C$:

$$\forall x \text{ in a neighborhood of } x_C, \quad Lf(x) = O(|x - x_C|^q).$$

(28)

The work presented here may be summarized as follows.

- We introduced three families of quasi-Trefftz functions for a class of 3D PDEs including the convected Helmholtz equation. Two of these, the GPWs, are generalizations of a PW ansatz, and were first introduced for a class of 2D problems. The ansatz defining these two families are defined in a neighborhood of a given point $x_C$ under the following forms: for all $x$,

\begin{align*}
J(x) := Q(x - x_C) \exp \Lambda \cdot (x - x_C) & \quad \text{for some polynomial } Q \text{ and some vector } \Lambda \in \mathbb{C}^3, \\
G(x) := \exp P(x - x_C) & \quad \text{for some polynomial } P.
\end{align*}

The third one is fully polynomial, and this is the first introduction and study of polynomial quasi-Trefftz functions. The corresponding ansatz is defined in a neighborhood of a given point $x_C$ under the following forms: for all $x$,

$$H(x) := R(x - x_C) \quad \text{for some polynomial } R.$$

- We provide explicit algorithms to construct quasi-Trefftz functions belonging to each of these three families, by constructing the corresponding polynomial $P$, $Q$ or $R$. This is achieved by a careful study of the system obtained by setting to zero the degree-$(q - 1)$ Taylor polynomial of the image of each ansatz through the operator $L$. It is then possible to choose adequately the degree of the polynomial $P$, $Q$ or $R$ in order to split this system into a hierarchy of linear triangular sub-system. Hence a solution to the system can be computed via an explicit formula by simply solving successively the subsystems by substitution. Interestingly, some of the polynomial coefficients of $P$, $Q$ and $R$ are free in the resulting algorithms, and thanks to these sets of linearly independent quasi-Trefftz functions can be constructed. As a consequence, beyond the construction of individual quasi-Trefftz functions, we can construct spaces of quasi-Trefftz functions.

- We prove that it is possible to construct quasi-Trefftz spaces $V_h$ spanned by sets of such quasi-Trefftz functions enjoying high order approximation property for exact solutions of the PDE. More precisely, given a given point $x_C$, Theorem 2 states that in order to achieve a given order of accuracy $n + 1$ of local approximation property in the following sense:

$$\forall u \text{ satisfying the governing PDE}, \exists u_a \in V_h \text{ s. t. } \|u - u_a\|_{L^\infty(B(x_C, h))} \leq Ch^{n+1},$$

(29)

where $B(x_C, h)$ denotes the sphere centered at $x_C$ of radius $h$ in $\mathbb{R}^3$; it is sufficient to construct a quasi-Trefftz space $V_h$ of dimension $p = (n + 1)^2$ with basis functions satisfying the quasi-Trefftz property (28) with $q = \max(n - 1, 1)$. For reference, reaching the same order of approximation in (29) using a standard polynomial space would yield a dimension $p = (n + 1)(n + 2)(n + 3)/6$ (corresponding to the full space of polynomials of degrees at most equal to $n$). For instance for $n = 8$ the quasi-Trefftz space is of dimension 81 while the polynomial space is of dimension 165. Besides, as noted in Theorem 2, we actually show a convergence in $H^1$:

$$\forall u \text{ satisfying the governing PDE}, \exists u_a \in V_h \text{ s. t. } \|u - u_a\|_{H^1(B(x_C, h))} \leq Ch^n.$$

(30)

Future plans include:
• first testing the approximation properties of the three families of quasi-Trefftz functions, in particular from the perspective of initialization of the construction process, conditioning of the resulting basis and stability in the high-frequency regime,
• then compare their performance with polynomial and wave-based bases - standardly used in the literature in aero-acoustics - in terms of accuracy, computing time and stability,
• finally comparing performance of a parallel implementation of quasi-Trefftz methods on realistic industrial test cases.

A A non-singular matrix statement

We will show here that under the assumption that $|M(x_C)| < 1$ then the matrix

$$C := \begin{bmatrix}
(M_1(x_C))^2 - 1 & \frac{1}{2}M_1(x_C)M_2(x_C) & \frac{1}{2}M_1(x_C)M_3(x_C) \\
\frac{1}{2}M_1(x_C)M_2(x_C) & (M_2(x_C))^2 - 1 & \frac{1}{2}M_2(x_C)M_3(x_C) \\
\frac{1}{2}M_1(x_C)M_3(x_C) & \frac{1}{2}M_2(x_C)M_3(x_C) & (M_3(x_C))^2 - 1
\end{bmatrix}$$

is not singular. For the sake of compactness we remove in this demonstration the dependency of the entries of $M$ on $x_C$.

First, we compute the determinant of $C$:

$$\det(C) = \left[ M_1^2 + M_2^2 + M_3^2 - 1 \right] + \left[ \frac{1}{2}(M_1M_2M_3)^2 - \frac{3}{4}(M_1^2M_2^2 + M_1^2M_3^2 + M_2^2M_3^2) \right].$$

We will prove that $\det(C) < 0$ by showing that both brackets in this last expression are negative, the first one strictly:

1. $1 > |M(x_C)|$ by assumption, so $[M_1^2 + M_2^2 + M_3^2 - 1] < 0$;
2. defining $a_1 = M_1^2M_2^2$, $a_2 = M_1^2M_3^2$ and $a_3 = M_2^2M_3^2$, then the following MacLaurin’s inequality:

$$\frac{a_1 + a_2 + a_3}{3} \geq \sqrt[3]{a_1a_2a_3}$$

shows that:

$$\frac{M_1^2M_2^2 + M_1^2M_3^2 + M_2^2M_3^2}{3} \geq |M_1M_2M_3|^{4/3},$$

combined with:

$$\begin{cases}
\frac{1}{2} \geq \frac{1}{3} \text{ and } 1 \geq \frac{1}{3} \\
|M_k|^{4/3} \geq |M_k|^2 \forall k \in \{1, 2, 3\} \text{ since } |M_k| < 1,
\end{cases}$$

in turn shows that:

$$\frac{M_1^2M_2^2 + M_1^2M_3^2 + M_2^2M_3^2}{2} \geq \frac{|M_1M_2M_3|^2}{3},$$

and therefore the second bracket in $\det(C)$ is negative:

$$\frac{1}{2}|M_1M_2M_3|^2 - \frac{3}{4}(M_1^2M_2^2 + M_1^2M_3^2 + M_2^2M_3^2) \leq 0.$$

This actually shows that $\det(C) < 0$, which indeed proves that the matrix $C$ is not singular.
B Spherical harmonics reminder

Legendre polynomials are defined on \( \mathbb{R} \) for \( m \in \mathbb{N}_0 \) as:

\[
P_l^m(x) = \frac{(-1)^m}{2^l l!} (1 - x^2)^{m/2} \partial_x^{l+m}(x^2 - 1)^l, \quad \forall x \in \mathbb{R},
\]

where the linear order \( \prec \) is defined by:

\[
x^0 \prec x^1 \prec \cdots \prec x^s \prec \cdots
\]

\( m \prec l \) if \( m - l \leq 0 \).

Moreover, for all \( l \) and \( m \) in \( \mathbb{N}_0 \) we note that:

\[
(x^2 - 1)^l = \sum_{l' = 0}^l \binom{l}{l'} (-1)^{l-l'} x^{2l'},
\]

\[
\partial_x^{l+m}(x^2 - 1)^l = \sum_{l' = \lceil \frac{l+m}{2} \rceil + 1}^l \binom{l}{l'} (-1)^{l-l'} \frac{(2l')!}{(2l' - l - m)!} x^{2l' - l - m}.
\]

As a result, from which we can write for all \( \theta \in \mathbb{R} \):

\[
\text{if } m \geq 0, P_l^m(\cos \theta) = \frac{(-1)^m}{2^l l!} (\sin \theta)^m \sum_{l' = \lceil \frac{l+m}{2} \rceil + 1}^l \binom{l}{l'} (-1)^{l-l'} \frac{(2l')!}{(2l' - l - m)!} (\cos \theta)^{2l' - l - m},
\]

\[
\text{if } m < 0, P_l^m(\cos \theta) = \frac{(l - |m|)!}{2^l l!(l + |m|)!} (\sin \theta)^m \sum_{l' = \lceil \frac{l+m}{2} \rceil + 1}^l \binom{l}{l'} (-1)^{l-l'} \frac{(2l')!}{(2l' - l - |m|)!} (\cos \theta)^{2l' - l - |m|}.
\]

C Faa di Bruno formula in 3D

In dimension three, the Faa di Bruno formula presented in [7] reads: if \( f \) is a function of one real variable and \( g \) is a function defined on \( \mathbb{R}^3 \), \( \forall x \in \mathbb{R}^3 \)

\[
\partial_x f(g(x)) = \sum_{1 \leq m \leq |i|} f^{(\bar{m})}(g(x)) \sum_{s=1}^{|i|} \frac{1}{p_s(i, \bar{m})} \prod_{m=1}^s \frac{1}{l_m!} \left( \frac{1}{l_m!} \partial_x^{l_m} g(x) \right)^{k_m}
\]

where the linear order \( \prec \) on \( \mathbb{N}_0^3 \) is defined in the introduction, while the partition \( p_s(i, \bar{m}) \) of multi-index \( i \in \mathbb{N}_0^3 \) is defined by:

\[
p_s(i, \bar{m}) = \left\{ (k_1, \ldots, k_s; l_1, \ldots, l_s); k_i > 0, 0 < l_1 < \cdots < l_s, \sum_{m=1}^s k_i = \bar{m}, \sum_{m=1}^s k_m l_m = i \right\}.
\]

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