Trefftz Functions for Nonlocal Electrostatics

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Abstract

Electrostatic interactions in solvents play a major role in biophysical systems. There is a consensus in the literature that the dielectric response of aqueous solutions is nonlocal: polarization depends on the electric field not only at a given point but in the vicinity of that point as well. This is typically modeled via a convolution of the electric field with an appropriate integral kernel.

A primary problem with nonlocal models is high computational cost. A secondary problem is restriction of convolution integrals to the solvent, as opposed to their evaluation over the whole space.

The paper develops a computational tool alleviating the “curse of nonlocality” and helping to handle the integration correctly. This tool is Trefftz approximations, which tend to furnish much higher accuracy than traditional polynomial ones. In the paper, Trefftz approximations are developed for problems of nonlocal electrostatics, with the goal of numerically “localizing” the original nonlocal problem. This approach can be extended to nonlocal problems in other areas of computational mathematics, physics and engineering.

1 Introduction

Electrostatic interactions are well known to play a major role in biomolecular and biophysical systems. For example, Ren et al. write in their review paper [55],

“Among the various components of molecular interactions, [electrostatic interactions] are of special importance because of their long-range nature and their influence on polar or charged molecules, including water, aqueous ions, proteins, nucleic acids, carbohydrates, and membrane lipids. In particular, robust models of electrostatic interactions are essential to understand the solvation properties of biomolecules and the effects of solvation upon biomolecular folding, binding, enzyme catalysis, and dynamics.”

Central in these models is an accurate representation of the dielectric properties of aqueous solutions. As e.g. Bardhan et al. note [11],

“One of the long-standing challenges in molecular biophysics is the development of accurate, yet simple models for the influence of biological fluids (aqueous solutions composed of water and dissolved ions) on biological molecules such as proteins and DNA.”

There is a consensus in the literature that accurate models of water and aqueous solvents must account for nonlocality. That is, in contrast to local descriptions, polarization $\mathbf{P}(\mathbf{r})$ and the displacement vector field $\mathbf{D}(\mathbf{r})$ depend on the electric field $\mathbf{E}$ not only at a given point $\mathbf{r}$, but in
the vicinity of that point as well. This dependence is usually expressed as convolution with an appropriate kernel (Section 2). The significance of nonlocal effects in the electrostatic response of solvents has been emphasized since the pioneering work of Dogonadze, Kornyshev, Vorotyntsev et al. in the 1970s [15,24,44]; see [9,10,34,58,69–71].

A primary problem with nonlocal models is high computational cost. In the Finite element (FE) or Finite Difference (FD) context, system matrices become less sparse by a factor of $O(\delta/h)^d$, where $\delta$ is the scale of nonlocal interactions, $h$ is the mesh size, and $d$ is the number of spatial dimensions. Note that dependence of the computational cost on the number of nonzero matrix entries is almost always superlinear.

A secondary problem is that convolution with the $E$ field should be confined to the nonlocal region (solvent); extending this convolution to the solute with local characteristics or to the whole space, as done in many existing publications, may lead to qualitatively incorrect results (Section 2.2).

The approach outlined in the paper is aimed at solving both principal problems: removing the computational “curse of nonlocality” and handling the convolution integrals properly. The main tool for that is Trefftz approximations, which in many instances furnish much higher accuracy than traditional piecewise-polynomial ones. This development is inspired by our successful application of Trefftz approximations in a variety of disparate problems: wave propagation and scattering, colloidal particles, photonic band structure, homogenization of periodic heterostructures [21,47,67,68]. At the same time, construction of Trefftz funtions for nonlocal problems is new (Section 3).

By definition, Trefftz functions satisfy locally (in weak form) the underlying differential equations of the problem. Examples of such functions are harmonic polynomials for the Laplace equation; plane, cylindrical or spherical waves for the Helmholtz or Maxwell equations, etc. The superior accuracy of Trefftz approximations explains their growing popularity in a large variety of methods and applications: Domain Decomposition [27,33], Generalized FEM [6,7,50,53,54,60], Discontinuous Galerkin (DG) [5,16,20,27,30,31,35,45], and FD (“Flexible Local Approximation MEthods,” FLAME) [61–65].

Trefftz functions derived in this paper can be incorporated into any of the above methods; the work on nonlocal Trefftz-FLAME and Trefftz-DG is planned. The key idea of FLAME is to replace the Taylor expansions on which classical FD is based with Trefftz approximations. This often leads to high-order schemes even in the presence of material interfaces [61–63,65–68].

DG-Trefftz methods possess many attractive features. Most relevant to the subject of this paper are exponential accuracy in many cases (Section 3.1, [37,45,46]); adaptivity [35,36]; a natural treatment of discontinuities – which is instrumental, in particular, for modeling solute-solvent interfaces. In general, DG methods can handle complex geometries, curved boundaries and various boundary conditions. Equations of Trefftz-DG reduce to the skeleton of the mesh, making the computation more efficient, since volume integrals vanish [25,45,46].
2 Nonlocal Electrostatics: Physical Models and Computational Complexity

2.1 Physical and Mathematical Models

2.1.1 Nonlocal Dielectric Properties

Nonlocal models, whereby one field at a given point depends on another field in the vicinity of that point, have been introduced in many areas of physics: plasticity, mechanical vibrations, liquid crystals, optics, nanostructures [1, 2, 4, 26, 41, 42, 48, 52, 59]. In the latter area, nonlocal treatment is particularly common in the description of plasmonic effects and in homogenization of metamaterials, where nonlocality often goes under the name of “spatial dispersion” (due to dependence of material parameters on the wave vector in Fourier space).

In macromolecular simulation, the importance of taking nonlocality into account is now widely recognized. As noted in the introduction, nonlocal electrostatic models were developed by Dogonadze, Kornyshev, Vorotyntsev and collaborators in the 1970s [15, 24, 44] and since then have been widely used and extended [9, 10, 12, 22, 34, 55, 57, 58, 69–71].

In linear local models the displacement field $\mathbf{D}$ is related to the electric field $\mathbf{E}$ as

$$\mathbf{D}(\mathbf{r}) = \varepsilon_l(\mathbf{r})\mathbf{E}(\mathbf{r})$$

where $\varepsilon_l$ is the dielectric permittivity of the medium and $\mathbf{r}$ is the position vector; linearity is assumed throughout the proposal. For simplicity, we also assume isotropy, which is accurate for aqueous solutions in the bulk, although the analysis and methods can be extended to anisotropic media if necessary.

It is important to distinguish convolution over the whole space $\mathbb{R}^d$ ($d = 1, 2, 3$) and the convolution-like integration restricted to a given domain $\Omega$; we denote the former and the latter with $\ast$ and $\ast_{\Omega}$, respectively:

$$\mathcal{E} \ast_{\Omega} \mathbf{E} \overset{\text{def}}{=} \int_{\Omega} \mathcal{E}(\mathbf{r} - \mathbf{r}')\mathbf{E}(\mathbf{r}')d\mathbf{r}'$$

The difference between integration over a bounded domain and the whole space does play a significant role (Section 2.2).

Nonlocal constitutive relation is assumed to have the form

$$\mathbf{D}(\mathbf{r}) = \varepsilon_l(\mathbf{r})\mathbf{E}(\mathbf{r}) + \varepsilon_{nl} \mathcal{E} \ast_{\Omega_{nl}} \mathbf{E}$$

where $\Omega_{nl}$ is the domain occupied by the nonlocal medium, and $\varepsilon_{nl}$ is a given parameter.

2.1.2 The Nonlocal Poisson Equation

In the chosen simply connected computational domain $\Omega$ with a Lipschitz-continuous boundary, the electrostatic potential $u$, the electric and displacement fields $\mathbf{E}$ and $\mathbf{D}$ satisfy

$$\mathbf{E} = -\nabla u; \quad \nabla \cdot \mathbf{D} = \gamma \rho; \quad u \in H^1(\Omega)$$

$\text{\footnotesize{1}}$Although the local term could be absorbed into the convolution integral as a Dirac delta function, it is expedient not to do so.
where $\rho$ is a given charge density and the coefficient $\gamma$ depends on the system of units.

Let $\Omega$ be partitioned into subdomains $\Omega_l$ and $\Omega_{nl}$ occupied by local and nonlocal media, where the respective constitutive relation are (1) and (3). On the interface boundary between $\Omega_l$ and $\Omega_{nl}$, the standard continuity condition for the normal component of $D$ holds:

$$D_{nl} \cdot n_{nl} + D_l \cdot n_l = 0$$

where $n_{nl}$ and $n_l$ are the outward unit normals to $\Omega_l$ and $\Omega_{nl}$, respectively, and the rest of the notation is self-explanatory.

### 2.1.3 The Poisson-Boltzmann Equation

Consider an electrolyte with positive and negative salt ions carrying equal and opposite charges. In general, there may be several species of ions; their statistical distribution in an electrostatic potential $u$ leads to the Poisson–Boltzmann equation (PBE) [17,23,28,29,32]:

$$\epsilon_s \nabla^2 u = -\rho - \sum_{\alpha} n_{\alpha} q_{\alpha} \exp\left(-\frac{q_{\alpha} u}{k_B T}\right)$$

where summation is over all species of ions present in the solvent, $n_{\alpha}$ is volume concentration of species $\alpha$ in the bulk, $q_{\alpha} = Z_{\alpha} e$ is the charge of species $\alpha$; $k_B$ is the Boltzmann constant, $T$ is temperature, and $\rho$ is the density of all charges other than the microions. If the electrostatic energy $q_{\alpha} u$ is much smaller than the thermal energy $k_B T$, then the PBE can be approximately linearized around $u = 0$ to yield

$$\epsilon_s \nabla^2 u - (k_B T)^{-1} \left(\sum_{\alpha} n_{\alpha} q_{\alpha}^2\right) u = 0$$

The potential satisfying this equation will typically exhibit exponential decay away from the sources. Eq. (7) can be extended to the nonlocal case by including the convolution term $\epsilon_{nl} \nabla \cdot (E^\ast_{\Omega_{nl}} \nabla u)$.

### 2.1.4 Limitations of the PBE Model

The main physical assumption behind the PBE is that each mobile charge is effectively in the mean field of all other charges, and has the Boltzmann probability of acquiring any given energy. This probability is assumed to be unconditional, i.e. not depending on possible redistribution of other ions in response to the motion of a given ion. In other words, mean field theory disregards any correlations between the positions and movement of the ions. However, it is demonstrated in [51] that such correlations may in fact be appreciable for multivalent ions. A consensus exists that at least for monovalent ions the correlations are weak enough for the PB model to be valid, and the linearized PBE (7) then provides a physically accurate description. The approach of this paper is extendable to the nonlocal version of the linearized PBE; Trefftz functions for that equation can be derived following the same procedure as for the nonlocal Poisson equation (Section 3).

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2Unit-dependent coefficients such as $4\pi$ or $\epsilon_0$ are for brevity omitted.
2.1.5 Solvent–Solute Boundary Value Problems (Nonlocal)

The formulation of solvent–solute boundary value problems is standard. Inside the solute (such as a macromolecule), the electrostatic potential is assumed to satisfy the classical Poisson equation

\[ \epsilon_m \nabla^2 u(r) = \gamma \rho_m(r), \]

where \( \epsilon_m \) is the (relative) dielectric permittivity of the molecule (typically assumed to be in the range from \( \sim 2 \) to 4), \( \rho_m(r) \) is the atomic charge density of the molecule (assumed to be given), and \( \gamma = 4\pi \) in the Gaussian system or \( \epsilon_0^{-1} \) in SI.

Within the solvent (domain \( \Omega_{nl} \)), in which the solute is immersed, and in the absence of charges, the electrostatic potential satisfies the nonlocal Laplace equation

\[ \nabla \cdot (E_{\Omega_{nl}} \nabla u) \equiv \nabla \cdot \int_{\Omega_{nl}} E(r - r') \nabla u(r') \, dr' = 0 \quad (8) \]

or, alternatively, the nonlocal Poisson-Boltzmann equation if microions are present. Across the solute-solvent interface, the potential is continuous, and so is the normal component of the \( D \) field. These boundary conditions are conventional, but in the solvent \( D \) is related to \( \nabla u \) nonlocally.

Numerical solution of the solvent–solute problem is facilitated by potential splitting, as \( \rho_m \) contains point charges which are difficult to handle numerically otherwise. Such splitting of the solution into the “forced” and “reaction” parts – in this case, \( u = u_f + u_r \) – is standard in the theory of differential equations, in wave scattering problems (incident + scattered fields), in magnetostatics \([67, \text{ Chap 10}]\), and in many other instances; \( u_f \) is the Coulomb potential of the given charges. Rather than applying the potential splitting in the whole space, it may be conceptually and algorithmically simpler to confine it to the solute. The resultant boundary conditions on the solute-solvent interface can be easily handled, especially in DG.

2.2 The Domain of Convolution Makes a Significant Difference

In most numerical procedures for the nonlocal electrostatic problem to date, the integration for the \( D \) field in (8) is extended from the solvent domain \( \Omega_s \) to the whole space, with the tacit physical assumption that this does not significantly affect the results. This extension is not just a matter of practical convenience; rather, it plays a critical role in the simplification of the problem.

Indeed, convolution-like integration over a fixed bounded domain, in contrast with integration over the whole space, does not possess several key properties and hence does not easily lend itself to simplification. First, “finite-domain convolution” is not in general commutative, a trivial example of which is

\[ 1 *_{[0,1]} x \equiv \int_0^1 1 \cdot x' \, dx' = \frac{1}{2} \neq x *_{[0,1]} 1 \equiv \int_0^1 (x - x') \cdot 1 \, dx' = x - \frac{1}{2} \quad (9) \]

Secondly, differentiation of finite-domain convolution does not in general reduce to differentiating either of the terms; e.g.

\[ d_x(x *_{[0,1]} 1) = d_x \left( x - \frac{1}{2} \right) = 1 \neq x *_{[0,1]} d_x 1 = 0 \quad (10) \]

Yet the localization method, proposed originally by Hildebrandt \([34, 69]\) and later developed, enhanced and implemented by others \([70–72]\), does rely on the standard differentiation rules for full-space convolutions (Section 2.3).

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\(^3\)The electronic charge density is accounted for via polarization – that is, via \( \epsilon_m \).
Remark. The bounded region of integration could be rigorously expanded to the whole space if the solution is padded with zero outside the computational domain. In that case, however, differentiation will be polluted by distributional derivatives (boundary delta functions).

Importantly, one may challenge the tacit assumption that extension of the convolution domain to the solute has only mild physical effects. As a simple illustration, we consider two closely related 1D problems on the interval \( \Omega = (-5, 5) \), with \( \Omega_{\text{nl}} = (-5, -1) \cup (1, 5) \), \( \Omega_l = (-1, 1) \):

\[
E_{1,2}(x) = -d_xu_{1,2}(x); \quad d_xD = 0 \quad (\Rightarrow D = \text{const})
\]

\[
D_{1,2}(x_0^+) = D_{1,2}(x_0^-), \quad x_0 = \pm 1; \quad u_{1,2}(-5) = 0; \quad u_{1,2}(5) = 1
\]

\[
D_1(x) = \mathcal{E} *_{\Omega} E_1 \equiv \int_{0}^{1} \mathcal{E}(x - x')E_1(x')dx'; \quad D_2(x) = \mathcal{E} *_{\Omega_{\text{nl}}} E_2 \equiv \int_{0}^{1} \mathcal{E}(x - x')E_1(x')dx'
\]

\[
\mathcal{E}(x) = \exp\left( -\frac{x^2}{2\sigma^2} \right), \quad \sigma = 1
\]

The two problems differ only in the domain of convolution with a Gaussian (for convenience) kernel. The results, however, are significantly different, as evident by the potential and field plots in Fig. 1, and by the fact that \( D_1 = D_1(x) \approx -0.3944 \), while \( D_2 \) is almost double that value, \( \approx -0.6553 \).

One concludes that the treatment of convolution, with the integration domain confined to the region of nonlocality \( \Omega_{\text{nl}} \), deserves closer attention.

From the physical perspective, one caveat is that the dielectric behavior of solvents in the vicinity of interfaces is not known well enough. Hence an objection may be raised that the mathematical model need not be more accurate than the available physical model. A possible response to this objection is three-fold. First, as the above 1D example illustrates, the treatment of nonlocal conditions might affect the solution not mildly and quantitatively, but qualitatively; this difference may prove to be critical for solvation problems, protein folding, and many other problems in biophysics. Second, it is of computational/mathematical interest to solve nonlocal problems efficiently and accurately. Third, if such accurate solutions are available, one may hope to start solving inverse problems – finding the best approximations to the dielectric function of the solvent near boundaries, although this ambitious goal is well beyond the scope of this paper.
2.3 The Hildebrandt Localization

An ingenious idea proposed by Hildebrandt et al. [34, 69] in the early 2000s and later enhanced and efficiently implemented by Xie et al. [70–72], allows one to convert nonlocal electrostatic problems to coupled local ones. This conversion is valid under the simplification assumptions noted below.

The essence of Hildebrandt’s approach can be explained as follows (technical details are available in the literature cited above). In the nonlocal region \( \Omega_{nl} \), we have

\[
\mathbf{D}(\mathbf{r}) = \mathcal{E} * \mathbf{E} = -\mathcal{E} * \nabla u \overset{!}{=} -\nabla (\mathcal{E} * u) \equiv -\nabla U, \quad U(\mathbf{r}) \overset{\text{def}}{=} \mathcal{E} * u, \quad \mathbf{r} \in \Omega_{nl} \tag{15}
\]

Thus \( U \) is the scalar potential for \( \mathbf{D} \) in \( \Omega_{nl} \). The governing equation for \( U \) in \( \Omega_{nl} \) therefore is

\[
-\nabla^2 U(\mathbf{r}) = \gamma \rho, \quad \mathbf{r} \in \Omega_{nl} \tag{16}
\]

The nonlocality has not yet been eliminated due to the nonlocal relation between \( u \) and \( U \). A critical simplification occurs for a specific but physically important class of convolution kernels. Namely, suppose that there exists a “magic” differential operator \( \mathcal{L} \) whose Green’s function is the given convolution kernel, i.e.

\[
\mathcal{L}\mathcal{E}(\mathbf{r}) = \delta(\mathbf{r}) \tag{17}
\]

Under that assumption, we obtain

\[
\mathcal{L}U = \mathcal{L}(\mathcal{E} * u) \overset{!}{=} (\mathcal{L}\mathcal{E}) * u = \delta * u = u \quad \text{in} \ \Omega_{nl}, \tag{18}
\]

where we used the fact that \( \mathcal{L} \) is a differential operator and that differentiation can be performed under the convolution sign. Thus the original nonlocal problem has been reduced to two local ones, (16), (18), coupled with the local problem within \( \Omega_l \) via the proper interface conditions between \( \Omega_{nl} \) and \( \Omega_l \). (Potential splitting noted above also needs to be incorporated in the actual procedure.)

A key issue is the transformations marked with the exclamation signs in (15) and (18). These transformations rely on the property of standard convolution over the whole space, but are invalid when integration is restricted to \( \Omega_{nl} \) (Section 2.2 and Remark therein).

3 Construction of Trefftz Functions for Nonlocal Electrostatics

3.1 Trefftz Approximations for the Laplace Equation: Harmonic Polynomials

Harmonic polynomials are known to provide an excellent (in some sense, even optimal [6]) approximation of harmonic functions [3, 6, 13, 49]. The following result is cited in [6]:

**Theorem 1.** (Szegö). Let \( \Omega \subset \mathbb{R}^2 \) be a simply connected bounded Lipschitz domain. Let \( \tilde{\Omega} \supset \supset \Omega \) and assume that \( u \in L^2(\tilde{\Omega}) \) is harmonic on \( \tilde{\Omega} \). Then there is a sequence \( (u_p)_{p=0}^\infty \) of harmonic polynomials of degree \( p \) such that

\[
\|u - u_p\|_{L^\infty(\Omega)} \leq c \exp(-\gamma p) \|u\|_{L^2(\tilde{\Omega})}
\]

\[
\|\nabla (u - u_p)\|_{L^\infty(\Omega)} \leq c \exp(-\gamma p) \|u\|_{L^2(\tilde{\Omega})}
\]

where \( \gamma, c > 0 \) depend only on \( \Omega, \tilde{\Omega} \).
Figure 2: Construction of Trefftz functions in a (small) 1D domain $\Omega_{\text{Trefftz}} \equiv (x_{\min}, x_{\max})$ indicated with a shaded rectangle. Only the $E$ field in $[0, x_{\max} + \delta]$ contributes to $D(x)$ in $\Omega_{\text{Trefftz}}$. Potential $u(x)$ is approximated by a set of basis functions (e.g. Taylor polynomials), and the expansion coefficients are determined by imposing, to a certain order, zero divergence conditions for $D$ in $\Omega_{\text{Trefftz}}$. See text for further details.

For comparison, the $H^1$-norm error estimate in standard FEM is

**Theorem 2.** (Ciarlet & Raviart, Babuska & Suri [19], [18], [8]). For a family of quasiuniform meshes with elements of order $p$ and maximum diameter $h$, the approximation error in the corresponding finite element space $V^n$ is

$$\inf_{v \in V^n} \| u - v \|_{H^1(\Omega)} = Ch^{\mu-1} p^{-(k-1)} \| u \|_{H^k(\Omega)}$$

where $\mu = \min(p + 1, k)$ and $c$ is a constant independent of $h$, $p$, and $u$.

Thus, for a fixed polynomial order $p$, the FEM and harmonic approximation errors are similar [6]; however, the FEM approximation is realized in a much wider space containing all polynomials up to order $p$, not just harmonic ones. For solving the Laplace equation, the standard FE basis set can thus be viewed as having substantial redundancy that is eliminated by using the harmonic basis.

*These results and observations motivate our development of Trefftz functions in the nonlocal case; we conjecture that similar excellent approximation properties will hold.* This is supported by the numerical experiments of Section 3.2.2.

### 3.2 Trefftz Functions for Nonlocal Problems

#### 3.2.1 1D Construction: Fixing Ideas

For simplicity of exposition, assume that the support of the convolution kernel is finite: $\text{diam}(\text{supp} \mathcal{E}) = \delta$ (if needed, all physically meaningful kernels in nonlocal electrostatics can be truncated with an exponentially small error). To fix ideas, let us start with a 1D setup (Fig. 2). Let $x > 0$ represent a nonlocal medium, and $x = 0$ be either the boundary of the computational domain or an interface boundary between local ($x < 0$) and nonlocal ($x > 0$) media.

The objective is to derive Trefftz functions $u_{\text{Trefftz}}(x)$ for a (small) interval $\Omega_{\text{Trefftz}} = (x_{\min}, x_{\max})$, indicated in Fig. 2 with a shaded purple rectangle. Assume that $x_{\min} < \delta$ (the case $x_{\min} > \delta$ is handled analogously and is slightly simpler). One observes that the $D$ field within $\Omega_{\text{Trefftz}}$ may depend only on the $E$ field within $[0, x_{\max} + \delta]$.

With this in mind, introduce a basis set $\{u_{\alpha}\}_{\alpha=0}^{n}$, $n$ being an adjustable parameter. An obvious, but not only, choice is the Taylor polynomials $u_{\alpha}(x) = (x - x_0)^\alpha$, where $x_0$ is an arbitrary point in $\Omega_{\text{Trefftz}}$. Then we have the respective functions

$$E_{\alpha}(x) = -d_x u_{\alpha}(x); \quad D_{\alpha}(x) = \int_{0}^{x_{\max} + \delta} \mathcal{E}(x - x') E_{\alpha}(x') \, dx'$$

(20)
Figure 3: One of the three Trefftz functions \( u(x) \) (left), with the corresponding \( E(x) \) (middle) and \( D(x) \) (right). Note the flatness of \( D(x) \) in the shaded vicinity of \( x_0 = 1 \). Parameters: \( \epsilon_l = 1, \epsilon_{nl} = 10, x_0 = 1, n = 4, m = 1 \); the Gaussian kernel with \( \sigma = 0.5 \).

Looking for \( u_{\text{Trefftz}} \) as a linear combination 
\[
u_{\text{Trefftz}}(x) = \sum_{\alpha=0}^{n} c_{\alpha} u_{\alpha}(x)
\]
and imposing conditions for the “1D divergence” of \( D \)
\[
d_{x}^{\beta} \text{div} D_{\text{Trefftz}}(x_0) \equiv \sum_{\alpha=0}^{n} c_{\alpha} d_{x}^{\beta} D_{\alpha}(x_0) = 0, \quad \beta = 1, 2, \ldots m
\] (21)
(where \( d_{x}^{\beta} \) is shorthand for \( d^{\beta}/d_{x}^{\beta} \)), one obtains Trefftz solutions whose number depends on the adjustable parameters \( n, m \). I call these solutions pseudoharmonic functions – by analogy with harmonic polynomials and “generalized harmonic polynomials” [37,49].

Plotted in Fig. 3 is one of the three pseudoharmonic functions for \( \epsilon_l = 1, \epsilon_{nl} = 10, x_0 = 1, n = 4, m = 1 \), and the Gaussian kernel \( E(x) = \exp(-x^2/(2\sigma^2)) \), \( \sigma = 0.5 \). Note the flatness of the \( D \) curve around \( x_0 = 1 \) (shaded area), as expected. Also note that in the nonlocal domain \( D \) is not proportional to \( E \).

This construction extends in a natural way to higher dimensions; the technical difficulties of computing convolution integrals exactly or approximately are overcome with the help of symbolic algebra (see the 2D example below).

While Trefftz sets are interesting in their own right, their main application is in the Trefftz-DG or Trefftz-FLAME context: then, \( \Omega_{\text{Trefftz}} \) will contain a given finite element, or a grid “molecule”. The Trefftz sets will in general vary from element to element or stencil to stencil, but that is a natural feature of both DG and FLAME. Importantly, one can then “forget” about nonlocality: information about it is built into the Trefftz functions, which can be used the same way as if the problem were local.

At an interface between nonlocal and local media, one additional step is required. Pseudoharmonic functions in the nonlocal medium must be glued with their local counterparts (typically, harmonic polynomials) via the matching conditions.

The pseudoharmonic functions constructed here should, strictly speaking, be classified as “quasi-Trefftz” [38–40], since they satisfy the underlying equation to a desired order rather than exactly. I still retain the plain term “Trefftz functions” for brevity, at the expense of a mild abuse of the terminology.\(^4\)

\(^4\)One may conjecture that the errors inherent in quasi-Trefftz functions can be ignored if they are of higher order than other numerical errors in a particular method. The “quasi” prefix can be restored in cases where it would make a difference.
Figure 4: A Trefftz function “in the bulk” of a nonlocal medium. Polynomial order for the potential $u(x, y)$ is $n_{\text{max}} = 4$. Gaussian kernel (in $x, y$) with $\sigma = \frac{1}{2}, \epsilon_l = 1, \epsilon_{nl} = 10$. Zero-divergence condition for $D$ imposed at $(x_0, y_0) = (0, 0)$ with partial derivatives up to order $m = 2$. Top row: potential $u_{\text{Trefftz}}$ and the corresponding $E_x, E_y$. Bottom row: $D_x, D_y$, and $\nabla \cdot D$.

### 3.2.2 2D Examples

In 2D, construction of pseudoharmonic functions is conceptually the same as in 1D. First, consider approximations “in the bulk” (i.e. away from any interfaces). As an illustrative example, let the domain $\Omega_a$, analogous to the one in Fig. 2, be $[-6\sigma, 6\sigma]^2$, with $\sigma = \frac{1}{2}$. Let the electrostatic potential $u$ be approximated in $\Omega_a$ by the set of all polynomials in $x, y$ up to order $n_{\text{max}} = 4$, leading to the respective fields $E = -\nabla u$ and $D = E \ast_{\Omega_a} E$, where $E$ is a Gaussian kernel in $x, y$ with the parameter $\sigma, \epsilon_l = 1, \epsilon_{nl} = 10$. Then impose conditions analogous to (21), with partial derivatives taken up to order $m = 2$ at $(x_0, y_0) = (0, 0)$. One of the Trefftz functions generated this way is shown in Fig. 4.

Exponential convergence of these Trefftz approximations with respect to the number of approximating functions (which in turn depends on the chosen polynomial order $n_{\text{max}}$) is illustrated by Fig. 5, in comparison with standard Taylor expansions. The approximation error is defined as

$$
\epsilon_a(V) \overset{\text{def}}{=} \inf_{u_a \in V} \| D_a(u_a) - D_{\text{test}} \|_V 
$$

where

- $D_a(u_a) = -E \ast_{\Omega_a} \nabla u_a$.
- $\Omega_t$ is the “target” domain for the condition $\nabla \cdot D \approx 0$. In the case of Trefftz approximations, $\Omega_t \equiv \Omega_{\text{Trefftz}}$. In the numerical example, $\Omega_t = (-\sigma, \sigma)^2$.
- $V = V(\Omega_t)$ is the approximating space, spanned either by the constructed Trefftz set or, alternatively, by Taylor polynomials of orders up to $n_{\text{max}}$. In the case of Taylor polynomials, the $x$ and $y$ components of $D$ are approximated separately, which arguably is an unfair advantage; yet convergence is still less rapid than in the case of Trefftz approximations.

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Figure 5: Error norms vs. the number of approximating functions. Trefftz approximation of $D_{\text{test}}$ is seen to converge much more rapidly than the standard Taylor expansion. $D_{\text{test},x} = \partial_y v_{\text{test}}$; $D_{\text{test},y} = -\partial_x v_{\text{test}}$; $v_{\text{test}} = \sin x \exp y + \exp(-x) \cos y$.

- In either case, $\|D\|_V^2 = \text{area}^{-1}(\Omega_t) \int_{\Omega_t} |D|^2 \, dx \, dy$
- A zero-divergence test function $D_{\text{test}}(x,y)$ is chosen as an example: $D_{\text{test},x} = \partial_y v_{\text{test}}$; $D_{\text{test},y} = -\partial_x v_{\text{test}}$; $v_{\text{test}} = \sin x \exp y + \exp(-x) \cos y$.

A more complicated example of a pseudoharmonic function in 2D is presented in Fig. 6. The kernel is Gaussian, with $\sigma = 0.5$; $\Omega_{\text{Trefftz}}$ is located at the origin, and the example also features a straight interface boundary $x = 0$ between the local (left) and nonlocal (right) media. In the local domain, the Trefftz functions are harmonic polynomials up to order 4. At the interface, the Trefftz functions satisfy the usual matching conditions for $u$ and $D \cdot n$; these are cumbersome but straightforward to impose using symbolic algebra; this only needs to be done once for any given integration kernel.

In practice, the computation of pseudoharmonic functions simplifies greatly if the convolution kernel $\mathcal{E}$ is separable or can be approximated as a combination of (a small number of) separable functions, since double integration reduces to a product of single integrals. Kernels commonly accepted in nonlocal electrostatics have the form of the Yukawa potential $\mathcal{E}(r, \lambda) = \frac{1}{4\pi \lambda^2} \exp\left(-\frac{r}{\lambda}\right)$ (single-pole in reciprocal space), where the $4\pi$ factor in the square brackets is present in the SI system but not in the Gaussian system, and parameter $\lambda$ defines the range of nonlocal interactions. Such singular kernels are not separable, and one has several options for finding pseudoharmonic functions:

(i) Consider separable approximations of the kernel; there is extensive literature on canonical tensor decomposition ([14, 43, 56] and references therein).

(ii) Precompute the Trefftz basis numerically and accurately; note that for any given kernel
Figure 6: Examples of 2D pseudoharmonic functions. Local and nonlocal regions: $x < 0$ and $x > 0$, respectively. Taylor order $n = 4$, $p_{\text{max}} = 2$. $\epsilon_l = 1$, $\epsilon_{\text{nl}} = 10$. Left: $u$, middle: $E_x$, right: $D_x$. Note that in the nonlocal domain $D$ is not proportional to $E$.

this needs to be done once. We previously implemented and used numerical Trefftz functions [21, Sect 5.1, 5.2] – this was done for local electrostatics, but the principle remains the same.

4 Conclusion

Trefftz functions, which, by definition, satisfy locally the underlying differential equation and applicable interface boundary conditions, tend to provide highly accurate approximations of the solution. This has led to the development of high-order Trefftz-FD schemes and Trefftz-DG methods with exponential convergence. Proposed in this paper is a way to generate Trefftz functions for nonlocal problems. Examples are presented, and exponential accuracy is demonstrated numerically.

In future research, Trefftz approximations are intended to be applied to problems of nonlocal electrostatics, important in biophysical and macromolecular simulation. It is anticipated that these approximations will help to alleviate the “curse of nonlocality” – much higher computational cost in comparison with local problems.

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