Discrete Green's function diakoptics : a toy problem

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Abstract — In Green’s function diakoptics, wavefield interactions between disjoint domains in space are described in terms of interacting multi-port subsystems. In addition to integral-equation based Green’s function diakoptics for time-harmonic fields, a demonstrably stable discrete space-time Green’s function diakoptics scheme has been reported to be effective for proximate regions. For distant regions it is necessary to retain a long field history. Upon considering a diakoptics toy problem involving two disjoint domains consisting of a single point each, the resulting boundary operator may be expressed in terms of two distinct discrete Green’s functions only, describing the intra- and inter-domain unit-source field responses, respectively.

There are various integral representations and asymptotic expansions for the discrete Z-domain Green’s functions, and it is even possible to construct representations for the discrete space-time Green’s functions consisting of nested finite sums, which turn out to be difficult to evaluate due to severe cancellations.

1 INTRODUCTION

One may describe wavefield interactions between disjoint domains in space in terms of interacting multi-port subsystems. This is referred to as diakoptics, and has been applied widely for time-harmonic fields, especially in combination with boundary integral equations (e.g., see [1] and references therein). However, its space-time-domain integral-equation based counterpart that remains stable has yet to be found.

We have previously reported on the construction of demonstrably stable time-domain finite-difference boundary conditions based on discrete Green’s function diakoptics for arbitrary bounded disjoint domains [2, 3]. These boundary conditions are effective for proximate regions. However, the more interesting case of distant regions is computationally more demanding, because a much longer time history sequence has to be retained. Here one has to realise that the associated discrete Green’s functions are much harder to evaluate than their continuous-space-time counterparts.

To get to the heart of the matter, we consider a diakoptics toy problem involving two disjoint domains, each consisting of a single point only. From our analysis, the role of the discrete Green’s will become manifest, prompting a brief review of integral representations and asymptotic expansions for the Z-domain discrete Green’s functions, and closed-form discrete-time expressions for special cases.

2 DISCRETE SPACE FIELD AND GREEN’S FUNCTIONS

Let us consider a time-discretised 0-form $\phi$ that formally assigns a time sequence of values to each of the vertices (nodes) of a simplicial complex [4]. In discrete electrodynamics the field variables are the 1-form $E$ and the dual 1-form $H$ that can be expressed in terms of discrete derivatives of the 0-form $\phi$ and the 1-form $A$. These potentials and the resulting fields are exact within the framework of the simplicial complex and its dual, which indicates the relevance of studying the 0-form $\phi$.

In the absence of sources $\phi$ satisfies the wave equation

$$\nabla \cdot (c^2 \nabla \phi) = 0,$$

where the operator $\nabla \cdot (c^2 \nabla)$ is the discrete counterpart of the Laplacian $\nabla \cdot \nabla$, $c$ denotes the wavespeed, and $\partial_t$ is some discrete time equivalent of the continuous time derivative operator, respectively.

Let us now specialise to the explicit FDTD case of a simple $\nu$-dimensional cubic lattice, scaled to unit grid size with central time differences. For simplicity, we adjust the time step $\Delta t$ and hence the Courant number $\alpha = \nu^{1/2}c\Delta t/h$ to the grid size $h = 1$ such that $\alpha = 1$. Further, we subject the field to a $Z$-transformation, according to $\phi(Z) = \sum_{n=0}^{\infty} \phi[n]Z^{-n}$, and introduce the negative mesh Laplacian $\nabla^2 = -*d*dd$. The 0-form field excited by a source distribution $q$ is the unique solution to the discrete Helmholtz equation in the absence of incident fields from infinity. For our diakoptics problem, we also require the 0-form discrete Green’s function excited by a unit-amplitude source located at the vertex $k_0$. The field
and the Green’s function respectively satisfy
\[ F \phi - \zeta \phi = q, \]
\[ FG - \zeta G = \delta_{k_0}, \]
where \( \zeta = \nu(2 - Z - Z^{-1})/\alpha \), and \( \delta_{k_0} = 1 \) at the vertex \( k_0 \) and \( \delta_{k_0} = 0 \) otherwise.

The Helmholtz equations for \( \phi \) and \( G \) are defined on an unbounded spatial grid, i.e., \( \mathbb{Z}^\nu \). However, in practice, one would like to perform computations on a bounded sub-domain of \( \mathbb{Z}^\nu \).

### 3 Exact Green’s Function Diakoptics Boundary Conditions

There are several ways of restricting finite-difference computations to a bounded sub-domain of \( \mathbb{Z}^\nu \), provided that that sub-domain is the discrete counterpart of a simply-connected domain (formally called a finitary 1-simply connected digital space [5]). If the pertaining sub-domain is convex, and embedded in a homogeneous background, absorbing boundary conditions may be quite effective. Amongst these the perfectly matched layers (PML) boundary conditions [6] have become the workhorse in many computational codes. As an alternative, Green’s-function based radiative boundary conditions have been applied successfully on an FDTD mesh [7], albeit that instability problems had to be overcome through an ad hoc suppression of the unstable eigenstates [8].

We have developed discrete Green’s function diakoptics for arbitrary bounded disjoint domains [3], with a view of confining the FDTD computations to domains of special interest, where for instance the evolution of non-linear generalised pseudospin field interactions may be simulated, while solving for the fields in the surrounding background medium in closed form. More specifically, let the computational domain \( D \) consist of two disjoint sub-domains with \( N \) mesh points in total. Upon arranging the field and the source distribution in \( N \)-dimensional vectors \( \phi \) and \( \mathbf{q} \), respectively, the finite-difference equations may be cast in the form
\[ S \phi = \mathbf{q} \quad \text{with} \quad S = P + F - \zeta I, \]
in which the \( P \) denotes the boundary operator that accounts for the influence of the homogeneous environment, and \( S \) and \( I \) denote the stability and identity operators, respectively. The action of the operator \( P \) is naturally restricted to the boundary points of \( D \).

To understand the issues at stake, it is instructive to consider a diakoptics toy problem involving two disjoint domains, each consisting of a single point, located at \( k_0 \) and \( k_1 \), respectively. There are several ways of constructing the boundary operator. For this toy problem, we define \( G_k \) as the field at \( k_1 \) due to a unit-amplitude source at \( k_0 \), or vice versa (by reciprocity), and \( G_0 \) as the field at \( k_0 \) (\( k_1 \)) due to a unit-amplitude source at \( k_0 \) (\( k_1 \)). Then, the source and the field solutions are simply given by
\[ \mathbf{q} = \begin{pmatrix} q_{k_0} \\ q_{k_1} \end{pmatrix}, \quad \phi = \begin{pmatrix} G_0 q_{k_0} + G_k q_{k_1} \\ G_k q_{k_0} + G_0 q_{k_1} \end{pmatrix}. \]

In view of translation symmetry and reciprocity, the matrix elements of \( S \) satisfy \( S_{11} = S_{22} = S_0 \), and \( S_{12} = S_{21} = S_k \), respectively. Hence, we may use Eq. (5) to solve \( S \phi = \mathbf{q} \) for \( S_0 \) and \( S_1 \). This leads to
\[ \begin{pmatrix} S_0 \\ S_1 \end{pmatrix} = \frac{1}{G_0^2 - G_k^2} \begin{pmatrix} G_0 & -G_k \\ -G_k & G_0 \end{pmatrix}, \]
and hence
\[ P = -\nu(Z + Z^{-1})I + \frac{1}{G_0^2 - G_k^2} \begin{pmatrix} G_0 & -G_k \\ -G_k & G_0 \end{pmatrix}, \]
where we have used \( 2\nu - \zeta = \nu(Z + Z^{-1}) \) for \( \alpha = 1 \).

As stated in [2], one may construct a Schwarz-formula based integral representation for \( P \) such that after discretisation the zeroes of the stability function end up on the unit circle in the complex \( Z \)-plane. This results in a self-consistent finite lookback scheme that is demonstrably stable in that only secular, non-growing, source-free solutions remain, which may be suppressed through the introduction of small losses.

One of the alternatives is to exploit causality by expanding the inverse of the stability function
\[ S^{-1} = \begin{pmatrix} G_0 & G_k \\ G_k & G_0 \end{pmatrix} \]
in terms of a power series in \( Z^{-1} \) and formally inverting the result. This results in a stable infinite lookback scheme involving matrix elements that may be generated on the fly. The details will be published elsewhere.

In any case, it is imperative that the pertaining Green’s functions are generated efficiently.

### 4 Green’s Function

The finite-difference \( Z \)-domain Green’s function \( G_k(Z) \) is closely related to the cubic lattice Green’s function \( q_k(w) \) that plays an important role in solid-state physics (here denoted in lowercase to avoid
confusion), and is defined as an integral over the \(\nu\)-dimensional (unit) torus \(T^\nu\)

\[
g_k(w) = \frac{1}{(2\pi)^\nu} \int_{T^\nu} \exp \left( i \sum_{m=1}^{\nu} k_m \theta_m \right) \sigma(\theta_1, \ldots, \theta_\nu, w) \, d^\nu \theta,
\]

which is analytic in the cut complex \(w\)-plane \(w \in \mathbb{C} \setminus [-\nu, \nu]\), and

\[
\sigma(\theta_1, \ldots, \theta_\nu, w) = w - \sum_{m=1}^{\nu} \cos \theta_m.
\]

The Green’s functions are related by \(G_k(Z) = g_k(w)/2\) with \(w = \nu(Z + Z^{-1})/2\). Over the years, a wide variety of techniques have been developed to analyse lattice Green’s functions. For the particular 3-dimensional cases of \((k_1, k_2, k_3) = (k, k, k)\) and \((k_1, k_2, k_3) = (2k, k, k)\), the body of knowledge is particularly deep [10, 11, 12].

Since \(g_k(w^*) = g_k(w)\), we may restrict our analysis to the lower half of the complex \(w\)-plane. Upon observing that

\[
\sigma^{-1} = i \int_0^\infty \exp(-i\sigma \tau) \, d\tau \quad \text{for} \ \text{Im}(w) < 0,
\]

we may rewrite Eq. (9) as (cf. Koster [9])

\[
g_k(w) = \frac{i}{(2\pi)^\nu} \int_0^\infty \exp \left( -i \rho \sigma + i \sum_{m=1}^{\nu} k_m \theta_m \right) \, d^\nu \theta \, d\tau.
\]

From Eq. (12) we may proceed in different directions. Evaluation of the integral over \(T^\nu\) yields [9]

\[
G_k(Z) = \frac{1}{2^\nu \pi^{3\nu}} \int_0^\infty \sum_{m=1}^{\nu} k_m \int_0^\infty e^{-i\omega \tau} \prod_{m=1}^{\nu} \frac{J_{k_m}(\tau)}{\sigma(\theta_1, \ldots, \theta_\nu, w)} \, d\tau,
\]

for \(\text{Im}(Z) < 0\). The reduction of a \(\nu\)-dimensional integral to a single Fourier integral comes at a cost, in that the integrand is more complex.

If the distance between the disjoint domains is large, Green’s function diakoptics is especially effective as compared to performing simulations on a finitary l-simply connected digital space that encloses the disjoint domains. Hence, we require sufficiently accurate expressions for \(G_k\) for large \(k\) (i.e., large \(\|k\|\)). Asymptotic expressions for arbitrary but large \(k\) have been derived from Eq. (12) to leading order [13]. For the special case of \((k_1, k_2, k_3) = (k, k, k)\) the full asymptotic expansion is available as well [10].

As an alternative to a quest for accurate and efficient methods for computing the lattice Green’s function in the \(Z\)-domain, we would be equally (or even more) content if we were able to evaluate the Green’s function in the discrete time domain. As pointed out in [4], we may use Eq. (3), and evaluate the operator \((F - I)^{-1}\) in terms of a series expansion in powers of \(Z^{-1}\). This requires careful bookkeeping. We provide two examples, viz.,

\[
G^{2n+1}_0 = \sum_{j=0}^{n} \sum_{j_1=0}^{j} \sum_{j_2=0}^{j_1} (-1)^{n+j_3-2j_1} \binom{n+j}{2j} \binom{2j}{j_1} \binom{2j_2}{j_2} \binom{2j_1}{j_1} \binom{2j_2}{j_2}
\]

for \(\nu = 3\),

\[
G^{2n+1}_k = \sum_{m=\ell}^{n} \sum_{j=0}^{m-\ell} (-1)^{m-n-2m-1} \binom{n+m}{2m} \binom{2m-2j-1}{m-j} \binom{2m+2j}{m-j-\ell}, \quad \text{for} \ k = (\ell, \ell),
\]

\[
G^{2n+1}_k = \sum_{m=\ell}^{n} \sum_{j=0}^{m-\ell} (-1)^{m-n-2m-1} \binom{n+m}{2m} \binom{2m-2j-1}{m-j-\ell}, \quad \text{for} \ k = (2\ell, 0)
\]

for \(\nu = 2\).

Although these expressions appear promising in that they only contain finite sums, loss of accuracy due to cancellations can play havoc with the results. For the 2D case, it is instructive to compare say \(G^{(15422,15422)}_{(15422,15422)} = 2.27 \times 10^{-3}\), which is the field on the diagonal at the wave arrival with \(G^{(15425)}_{(15421,0)}\) chosen because \(15422 + 15422 \approx 15421\). Unfortunately, the expression in Eq. (15) evaluated in quadruple precision yields a staggering \(-2.29 \times 10^{2181}\) for the latter. We would have to work with about 2525 significant digits to get the result for this example right. The 3D case is considerably more difficult. The numerical example above demonstrates that an alternative representation for \(G^{2n+1}_k\) is required.

5 CONCLUSIONS

We have demonstrated that the boundary operator for a diakoptics toy problem involving two disjoint single-point domains may be expressed in terms of two distinct discrete Green’s functions only, describing the intra- and inter-domain unit-source field responses, respectively.

In view of their importance of the Green’s functions, we have reviewed two alternative integral representations for the \(Z\)-domain discrete Green’s functions, and have discussed the existence of asymptotic expansions for large distances. We have presented special cases for the closed-form nested
finite-sum representations for the discrete space-time Green’s functions. Although those expressions seem straightforward, their usefulness is restricted due to numerical cancellations.

References


[10] G S Joyce and R T Delves, “Exact product forms for the simple cubic lattice Green func-


