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Interpolation of 2D Layered-Medium Periodic Green's Function

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Introduction

An important problem in many applications is the efficient computation of the two-dimensional (2D) periodic Green's functions in layered media. In this paper, we investigate various ways to use interpolation to speed up the calculation of the periodic 2D Green's function in layered media. This corresponds to the calculation of the potential from a 2D infinite periodic set of source points arranged on a lattice in the xy plane, with z being the direction normal to the layers. The lattice vectors s_1 and s_2 in the plane of the sources may be arbitrary, corresponding to a skewed lattice as illustrated in Fig. 1.
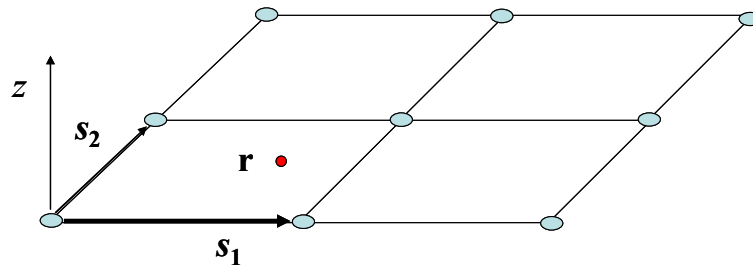

Figure 1. Geometry of an infinite 2D lattice of source points on a general skewed lattice in the xy plane, residing within a layered medium (layers not shown). An observation point r within the (0,0) unit cell at an arbitrary z is also shown.

In layered media, the 2D periodic Green's function has a spectral representation of the form

$$G(\mathbf{r},\mathbf{r}') = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \tilde{G}_{pq}(\mathbf{r},\mathbf{r}'), \tag{1}$$

where the sum is over spectral components $\tilde{G}_{pq}$. When the source and observation points are in the same or adjacent layers, in order to accelerate the computation the asymptotic forms of $\tilde{G}_{pq}$ are typically removed from the Green's function to regularize it. The removed terms represent direct and quasi-image contributions (i.e., first-bounce reflections from interfaces adjacent to the source layer). The removed terms, corresponding to 2D periodic Green's functions in a homogeneous media, are added back in a form that is itself accelerated using the Ewald method [1–3]. The Ewald method uses a representation for the homogeneous medium periodic Green's function that is a sum of a "modified spectral" and "modified spatial" series. Each one is a rapidly converging sum, exhibiting Gaussian convergence. The resulting Green's function representation may be written as

$$G(\mathbf{r},\mathbf{r}') = G^{reg}(\mathbf{r},\mathbf{r}') + G^{\text{Ewald}}_{\text{spatial}}(\mathbf{r},\mathbf{r}') + G^{\text{Ewald}}_{\text{spectral}}(\mathbf{r},\mathbf{r}'). \qquad (2)$$

The regularized Green's function is non-singular at the lattice source points when the lattice is embedded within a layer; when the lattice is at an interface there still exists a low-order singularity, but at least the potentials are finite at the lattice source points. In either case, the regularized periodic Green's function is much smoother and therefore more amenable to interpolation than the "unregularized" form [4]. Furthermore, the regularized Green's function can be computed much faster than the "unregularized" one, since the subtraction of the homogenous-medium terms accelerates the convergence.

Here we propose two uses of interpolation, of which the first is a direct interpolation technique applied to the regularized Green's function. This requires a four-dimensional interpolation in the space domain, namely, in the variables x-x', y-y', z and z'. To further enhance the speed-up, a three-dimensional interpolation is applied to the extracted parts (homogeneous-medium periodic Green's functions, which are evaluated by the Ewald method) after they are regularized by extracting contributions from the four corner source terms in the (0,0) unit cell containing the observation point.

4D Interpolation for the regularized Green's function

Using the periodic property of the regularized Green's function, we need only interpolate observation points within a single unit cell, assumed to be the (0,0) unit cell. For observation points outside the unit cell, the observation point is shifted an integral number of lattice periods into the unit cell, with the result multiplied by a progressive phase shift term corresponding to the number of lattice periods translated in each dimension. Since even the "regularized" Green's function components typically have slope discontinuities across the interfaces, one should not interpolate across media interfaces. Furthermore, different sampling densities may also be needed in different layers. Hence, a separate set of tables must be maintained for every combination of source-point and observation-point layers.

A simple, three-point (quadratic) interpolation in the four variables (x-x', y-y', z and z'), for example, requires $3^4 = 81$ interpolation points. Rather than using the conventional 81-point scheme, a 4D simplex scheme is employed that reduces the number of interpolation points to as low as 15, resulting in a further speed-up with no sacrifice in accuracy.

3D interpolation for extracted terms (Ewald terms)

The extracted terms (the terms extracted from the total Green's function to regularize it) correspond to 2D periodic Green's functions in a homogeneous medium. These are calculated using the Ewald method. Although the Ewald method is a very powerful method to calculate the 2D periodic homogenous-medium Green's function, especially when the vertical separation z-z' is relatively small, the calculation of this Green's function may also be speeded up by using interpolation. The Ewald formulation is a hybrid method resulting in two series, namely a spatial and a spectral series. The Ewald spectral series is regular at the periodic source points, while the Ewald spatial series has singularities at the source points. If the spatial Ewald series is regularized, then the sum of the two series is regularized and the resulting smoothing greatly facilitates

interpolation. The spatial series is regularized by removing the contributions from the four corner sources of the (0,0) unit cell that contains the observation point. Interpolation of the regularized Ewald series (i.e., the regularized Ewald spatial series added to the Ewald spectral series) requires a set of 3D interpolation tables since it has functional dependencies on x-x', y-y' and z-z'. Using this method, a speed-up factor of about 8 has been observed for the calculation of the 2D periodic homogenous-medium Green's function using a simple quadratic interpolation with $3^3 = 27$ interpolation points. A better speed-up factor of about 13 was gained by interpolating on a 3D simplex with 10 interpolation points. The 3D simplex is shown in Fig. 2.
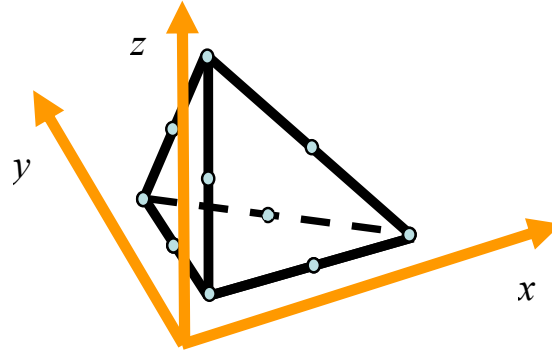

Figure 2. Geometry of a simplex in 3D for quadratic interpolation.

Numerical Results

A combination of 3D and 4D interpolations has been explored for accelerating the computation of the 2D periodic Green's function in a layered medium. The method involved two steps, where the first step is regularization of the function and the second step is interpolation. The interpolations described above were implemented in the simulation tool EIGER™ (Electromagnetic Interactions Generalized) [5]. Various geometries have been tested with and without interpolation in order to observe the resulting speed-up while maintaining a desired accuracy.

Table 1 presents some results for the simple test case of a 2D periodic array of perfectly conducting rectangular patches. The patch lying within the unit cell is rather finely gridded so that it has a relatively large number of basis functions, i.e., degrees of freedom (DOFs). Five different meshes were used, with varying numbers of DOFs. The first column of the table shows the number of DOFs on the unit-cell patch for that particular mesh. For each DOF, the first row in Table 1 indicates timing results with no interpolation, whereas the second and the third rows are with interpolation using 5×5 and 10×10 interpolation points within the unit cell, respectively. The second column gives the times needed to evaluate the Green's functions. (For the interpolation cases shown in the second and third rows for each DOF, this corresponds to the times needed to set up the interpolation tables.) The third column shows the actual times spent doing interpolation. The fourth column gives the time consumed in performing the necessary inner products between basis and testing functions. The fifth column gives the time to solve the moment-method system of equations. The last column is the total time.

As the last column indicates, more DOFs result in greater speed-up factors since the time to build up the interpolation tables is almost constant. Speed-up factors as high as about 70 are observed in this particular example. Even for the 5×5 interpolation grid case, the solution was accurate to better than 0.1% error, compared with the reference solution (no interpolation).

Table 1. Comparison of computation times.

DOF	Green's Fn. Time (sec)	Interpolation Time (sec)	Inner Product Time (sec)	Solution Time (sec)	TOTAL Time (sec)
8	12.828	--------	0.0575	6.25E-04	12.921
	0.2753	0.1428			0.4687
	0.7414	0.1428			0.8906
50	249.17	--------	0.9734	6.72E-03	251.12
	0.2753	2.7076			3.9375
	0.7414	2.7076			4.3750
200	1502.1	--------	5.3471	0.2005	1509.6
	0.2753	16.300			22.172
	0.7414	16.300			22.734
450	5527.3	--------	22.093	2.1067	5553.1
	0.2753	58.309			79.609
	0.7414	58.309			80.625
800	14403	--------	44.328	11.672	14482
	0.2753	151.10			206.02
	0.7414	151.10			208.45

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