SCUFF-STATIC: Pure Electrostatics in SCUFF-EM

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1 Overview

The core SCUFF-EM library is designed to solve electromagnetism problems at nonzero frequencies. In principle, we can use it to solve electrostatics problems simply by working at low nonzero frequencies and extrapolating to the $\omega \to 0$ limit. This approach works adequately in many cases of interest (as, for example, in the "electrostatics of a spherical dielectric shell" example on the SCUFF-EM website.[1])

However, there are at least two drawbacks to such an approach:

- The nonzero-frequency BEM formulations used by LIBSCUFF are solving for surface *currents* (both electric and magnetic currents), whereas for electrostatics problems the appropriate unknowns are electric *charges* with no magnetic unknowns. Because there are multiple current distributions whose divergence yields the same charge density, the full-wave formulations in LIBSCUFF become ill-conditioned in the extreme DC limit. Even for low-but-not-extremely-low frequencies at which the full-wave formulation is not particularly badly behaved, it is still computationally *wasteful* to solve for electric and magnetic currents when we only need electric charges. Indeed, for a dielectric object represented by a surface mesh of N triangular panels, the full-wave formulation of LIBSCUFF involves roughly $3N$ unknowns, whereas a pure-electrostatics formulation requires exactly N unknowns, as discussed below.

- In electrostatics we frequently encounter boundary conditions consisting of fixed potentials on conductor surfaces. This kind of boundary condition is unwieldy to support in core LIBSCUFF (although the SCUFF-RF module does support a version of it in the definition of port voltages).

To address these difficulties, SCUFF-EM includes a pure electrostatics module known as SCUFF-STATIC. This code reuses much of the existing LIBSCUFF infrastructure to implement an electrostatic BEM formulation. It is designed to be easily incorporated into existing SCUFF-EM workflows; in particular, it reads the same `.scuffgeo` files for describing geometries.[2] The following section of this memo describes the (standard) electrostatic BEM formulation used by SCUFF-EM, and subsequent sections discuss the implementation of the various types of calculation you can request in a SCUFF-STATIC run.

Implementation of λ-surfaces

In addition to the usual electrostatic boundary conditions for perfect conductors and dielectrics, SCUFF-STATIC supports an exotic type of boundary condition

[1] `http://homerreid.com/scuff-EM/scuff-scatter/scuffScatterExamples.shtml#SphericalShell`.

[2] One distinction: SCUFF-STATIC does not presently support `LATTICE` statements, i.e. extended objects with periodic boundary conditions.

that I will call "λ-conditions," which arises in theoretical treatments of entanglement entropy. At a point $\mathbf{x}$ on the surface of a body satisfying λ-conditions (which I will call a "λ-surface"), the boundary condition on the electrostatic potential is

$$\left|\frac{d\phi}{d\hat{\mathbf{n}}}\right|_{\mathbf{x}^+} - \left|\frac{d\phi}{d\hat{\mathbf{n}}}\right|_{\mathbf{x}^-} = \frac{1}{\lambda}\phi(\mathbf{x}) \tag{1}$$

where λ is a material property of the surface. [Noting that the LHS of (1) is the jump in normal electric field across the two sides of a surface in vacuum, it is tempting to interpret the RHS as a surface charge density, in which case we can think of $1/\lambda$ as a sort of linear semiconducting susceptibility, i.e. the surface develops a local charge density proportional to the local electrostatic potential with proportionality constant $1/\lambda$.] λ-surfaces are described in SCUFF-EM geometry files as infinitesimally thin objects whose dielectric constant has zero real part and negative imaginary part; the absolute value of the imaginary part is taken as the value of λ.

2 Theory

As in the usual LIBSCUFF, we imagine geometries to consist of homogeneous regions $\{\mathcal{R}_r\}$. Homogeneous region $\{\mathcal{R}_r\}$ has relative dielectric permittivity ϵ_r.

The boundary of $\mathcal{R}_r$ is denoted $\partial\mathcal{R}_r$; it may consist of a single closed surface or a union of surfaces, each of which may be individually open. Thus we write

$$\partial\mathcal{R}_r = \cup\mathcal{S}_s \tag{2}$$

Each surface $\mathcal{S}_s$ bounds precisely two regions; thus $\mathcal{S}_s$ appears on the RHS of equation (2) for two different values of r.

On each surface lives a surface charge density $\sigma(\mathbf{x})$.

Surface $\mathcal{S}_s$ may optionally be PEC, in which case it must be assigned a fixed potential V_s before the problem can be solved. Physically, a PEC surface corresponds to an infinitesimally thin conducting layer at the interface between two dielectric regions, and the surface charge on such a surface represents free charges supplied to the surface by whatever batteries initially charged them up to their specified potentials V_s.

On the other hand, a non-PEC surface simply desribes the interface between two dielectric regions, and the surface charge on such a surface represents the divergence of the bound volume polarization density in the dielectric region. Among other things, this means that the total surface charge integrated over the boundary of a dielectric region must vanish. There is no such constraint on the total surface charge on PEC surfaces.

Potentials and fields from charge densities: continuous forms

The electrostatic potential and field at an arbitrary point $\mathbf{x}$ are obtained by summing contributions from surface charges on all surfaces, plus the contributions of any external field sources that may be present:

$$\phi(\mathbf{x}) = \phi^{\rm ext}(\mathbf{x}) + \frac{1}{4\pi\epsilon_0}\sum_s \oint_{\mathcal{S}_s} \frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\sigma(\mathbf{x}')\,d\mathbf{x}' \tag{3a}$$

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}^{\rm ext}(\mathbf{x}) + \frac{1}{4\pi\epsilon_0}\sum_s \oint_{\mathcal{S}_s} \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3}\,\sigma(\mathbf{x}')\,d\mathbf{x}'. \tag{3b}$$

where $\phi^{\rm ext}, \mathbf{E}^{\rm ext}$ are the potential and field due to external field sources.[3]

There are several important distinctions between these equations and the corresponding equations in the full-wave formulations:

- The integrals in (3) are over *all* surfaces in the problem, not just the surfaces bounding the region in which the evaluation point lies. This is in contrast to the full-wave case, in which the corresponding surface integrals range only over the surfaces bounding the medium in question.

[3] In a full-wave scattering problem these would be the "incident" fields, but in an electrostatic problem the word "incident" doesn't quite make sense, so we call them the "external" fields instead.

- Similarly, $\phi^{\rm ext}, \mathbf{E}^{\rm ext}$ contribute to the total fields at *all* points in space, not just points living in the same regions as the external field sources. This is again in contrast to the full-wave case, where the incident field sources contribute only to fields at points in the same region as those sources.
- Equations (3) do *not* involve the dielectric constants of the various regions. Instead, surface charges on all surfaces contribute to the potential as they would in vacuum. The dielectric constants of the various materials enter only through the boundary conditions, discussed below.
- Another distinction with the full-wave case which is not apparent from (3) is that we can have nonzero induced charge densities σ even in the absence of any external fields. This is possible if the problem involves conducting surfaces maintained at nonzero potentials.

Surface charge density expansion

Now imagine approximating surface $\mathcal{S}_s$ as the union of $N_s^{\rm P}$ flat triangular panels,

$$\mathcal{S}_s = \cup \mathcal{P}_{sa}$$

where $a = 1, \cdots, N_s^{\rm P}$. Let P_{sa} have area A_{sa} and surface normal $\hat{\mathbf{n}}_{sa}$. (We will worry about the direction of $\hat{\mathbf{n}}_{sa}$ later.)

To panel $\mathcal{P}_{sa}$ we assign a scalar-valued "pulse" basis function $b_{sa}(\mathbf{x})$ that is 1 on the panel and 0 elsewhere:

$$b_{sa}(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in \mathcal{P}_{sa} \\ 0, & \text{otherwise.} \end{cases}$$

We approximate the surface charge density on $\mathcal{S}_s$ as an expansion in the b_{sa} functions:

$$\frac{\sigma(\mathbf{x})}{\epsilon_0} \approx \sum_{a=1}^{N_s^{\rm P}} \sigma_{sa} b_{sa}(\mathbf{x}) \qquad \text{for } \mathbf{x} \in \mathcal{S}_s.$$

Note that my σ_{sa} unknowns have the dimensions of

$$\frac{\text{surface charge density}}{\text{permittivity}} = \frac{\text{volts}}{\text{length}}.$$

In what follows, I will frequently use the collective subscript $n = (sa)$ with $\sum_n = \sum_s \sum_a$, i.e. a sum over n runs over all panels on all surfaces.

Potentials and fields from charge densities: discretized forms

The electrostatic potential and field at $\mathbf{x}$ are

$$\phi(\mathbf{x}) = \phi_r^{\rm ext}(\mathbf{x}) + \sum_n \sigma_n \int_{\mathcal{P}_n} \frac{d\mathbf{x}'}{4\pi|\mathbf{x}-\mathbf{x}'|} \tag{4a}$$

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}_r^{\rm ext}(\mathbf{x}) + \sum_n \sigma_n \int_{\mathcal{P}_n} \frac{(\mathbf{x}-\mathbf{x}')d\mathbf{x}'}{4\pi|\mathbf{x}-\mathbf{x}'|^3} \tag{4b}$$

where the sum is over all panels on all surfaces in the problem.

Conditions on potentials and fields

Conditions at PEC surfaces

At PEC surfaces we impose the condition that the electrostatic potential equal the specified potential for that conductor:

$$\phi(\mathbf{x}) = V_s, \qquad \text{for } \mathbf{x} \in \mathcal{S}_s.$$

Galerkin-testing with the expansion functions for surface $\mathcal{S}_s$, we find

$$\int_{\mathcal{P}_{sa}} \phi(\mathbf{x}) d\mathbf{x} = A_{sa} V_s, \qquad \text{for all panels } \mathcal{P}_{sa} \text{ on surface } \mathcal{S}_s.$$

Inserting (4a), this reads

$$\sum_n \mathcal{I}^{(1)}_{mn} \sigma_n = A_m V_m - \int_{\mathcal{P}_m} \phi^{\text{ext}}(\mathbf{x}) d\mathbf{x} \tag{5}$$

where V_m is the potential at which the conducting surface containing panel $\mathcal{P}_m$ is held and

$$\mathcal{I}^{(1)}_{mn} \equiv \int_{\mathcal{P}_m} \int_{\mathcal{P}_n} \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}\, d\mathbf{x}'\, d\mathbf{x}.$$

Conditions at dielectric surfaces

At non-PEC surfaces we impose the condition that the normal electric field exhibit the requisite discontinuity. If $\mathbf{x}$ is a point on a surface $\mathcal{S}_s$ lying between regions $\mathcal{R}_r$ and $\mathcal{R}_{r'}$, the condition is

$$\epsilon_r \left| \frac{\partial \phi}{\partial \hat{\mathbf{n}}} \right|_{\mathbf{x}^+} = \epsilon_{r'} \left| \frac{\partial \phi}{\partial \hat{\mathbf{n}}} \right|_{\mathbf{x}^-} \tag{6}$$

where $\hat{\mathbf{n}}$ is the surface normal pointing away from $\mathcal{R}_r$ into $\mathcal{R}_{r'}$, and where x^+ and x^- are points lying infinitesimally displaced from $\mathbf{x}$ along $\hat{\mathbf{n}}$ into $\mathcal{R}_r$ and $\mathcal{R}_{r'}$.

When we seek to enforce condition (6) at a point $\mathbf{x}$ lying within a panel $\mathcal{P}_{sa}$ on $\mathcal{S}_s$, we find the following dichotomy:

1. Surface charges on $\mathcal{P}_{sa}$ contribute to the two sides of (6) with *opposite* signs.

2. Surface charges on all other panels, as well as the external field sources, contribute to the two sides of (6) with the *same* sign.

Equation (6) thus reads, for a point $\mathbf{x}$ on $\mathcal{P}_m$,

$$\epsilon_r \left[\frac{\sigma_m}{2} + \sum_{n\neq m} \sigma_n \int_{\mathcal{P}_n} \frac{\hat{\mathbf{n}}_m \cdot (\mathbf{x}-\mathbf{x}')}{4\pi|\mathbf{x}-\mathbf{x}'|^3}\, d\mathbf{x}' + \hat{\mathbf{n}}_m \cdot \mathbf{E}^{\rm ext}(\mathbf{x}) \right]$$
$$= \epsilon_{r'} \left[-\frac{\sigma_m}{2} + \sum_{n\neq m} \sigma_n \int_{\mathcal{P}_n} \frac{\hat{\mathbf{n}}_m \cdot (\mathbf{x}-\mathbf{x}')}{4\pi|\mathbf{x}-\mathbf{x}'|^3}\, d\mathbf{x}' + \hat{\mathbf{n}}_m \cdot \mathbf{E}^{\rm ext}(\mathbf{x}) \right]$$

or

$$\sigma_m + \Delta_{rr'} \sum_{n\neq m} \sigma_n \int_{\mathcal{P}_n} \frac{\hat{\mathbf{n}}_m \cdot (\mathbf{x}-\mathbf{x}')}{4\pi|\mathbf{x}-\mathbf{x}'|^3}\, d\mathbf{x}' = -\Delta_{rr'} \hat{\mathbf{n}}_m \cdot \mathbf{E}^{\rm ext}(\mathbf{x}) \tag{7}$$

with

$$\Delta_{rr'} = 2\frac{\epsilon_r - \epsilon_r'}{\epsilon_r + \epsilon_r'}. \tag{8}$$

Now Galerkin-test (7) with the pulse basis function associated with panel m:

$$A_m \sigma_m + \Delta_{rr'} \sum_{n\neq m} \mathcal{I}^{(2)}_{mn} \sigma_n = -\Delta_{rr'} \int_{\mathcal{P}_m} \hat{\mathbf{n}}_m \cdot \mathbf{E}^{\rm ext}(\mathbf{x}) d\mathbf{x} \tag{9}$$

where

$$\mathcal{I}^{(2)}_{mn} \equiv \int_{\mathcal{P}_m} \int_{\mathcal{P}_n} \frac{\hat{\mathbf{n}}_m \cdot (\mathbf{x}-\mathbf{x}')}{4\pi|\mathbf{x}-\mathbf{x}'|^3}\, d\mathbf{x}'\, d\mathbf{x}.$$

Conditions at $\lambda-$ surfaces

As a generalization of the usual electrostatics for PEC and dielectric bodies, SCUFF-STATIC also supports a modified type of boundary conditions that we will call λ-*conditions*. The λ boundary condition is defined by

$$\lambda \left\{ \left| \frac{d\phi}{d\hat{\mathbf{n}}} \right|_{\mathbf{x}^+} - \left| \frac{d\phi}{d\hat{\mathbf{n}}} \right|_{\mathbf{x}^-} \right\} = \phi(\mathbf{x}). \tag{10}$$

Surfaces satisfying λ conditions will be known as λ-*surfaces*. We may think of λ-surfaces as a type of semiconducting surface on which reside a surface charge density proportional to the local electrostatic potential.

It's easy to write down the Galerkin-tested version of (10). Consider testing each side with the pulse basis function associated with panel m. By the dichotomy discussed above, the contribution of all other panels $\mathcal{P}_{n\neq m}$ to the quantity in curly brackets vanishes, as does the contribution of the external field. The contribution of $\mathcal{P}_m$ may be evaluated in a way similar to our evaluation of the diagonal matrix element in the dielectric case discussed above. The Galerkin test of the RHS proceeds similarly to our discussion of the PEC case above. We obtain

$$\lambda A_m \sigma_m - \sum_{mn} \mathcal{I}^{(1)}_{mn} \sigma_n = \int_{\mathcal{P}_m} \phi^{\rm ext}(\mathbf{x})\, d\mathbf{x}.$$

BEM system

Assembling equations (5) for PEC panels, (9) for all dielectric panels, and (10) for all λ panels into a big linear system, we have

$$\mathbf{M}\boldsymbol{\sigma} = \mathbf{v} \tag{11}$$

where the mth entry of the unknown vector σ is the surface charge density (divided by ϵ_0) on the mth panel, and where the elements of the BEM matrix and the RHS vector are

If panel m is on a PEC surface:

$$M_{mn} = \mathcal{I}^{(1)}_{mn}, \qquad\qquad v_m = A_m V_m - \int_{\mathcal{P}_m} \phi^{\text{ext}}(\mathbf{x})\, d\mathbf{x}.$$

If panel m is on a dielectric surface:

$$M_{mn} = \begin{cases} A_m, & m = n \\ \Delta_{rr'}\mathcal{I}^{(2)}_{mn}, & m \neq n \end{cases} \qquad v_m = -\Delta_{rr'} \int_{\mathcal{P}_m} \hat{\mathbf{n}}_m \cdot \mathbf{E}^{\text{ext}}(\mathbf{x})\, d\mathbf{x}.$$

If panel m is on a λ-surface:

$$M_{mn} = \lambda A_m \delta_{mn} - \mathcal{I}^{(1)}_{mn}, \qquad v_m = + \int_{\mathcal{P}_m} \phi^{\text{ext}}(\mathbf{x})\, d\mathbf{x}.$$

In these equations,

- V_m denotes the potential at which the conducting surface containing panel $\mathcal{P}_m$ is held.
- $\Delta_{rr'}$ is quantity (8) with ϵ_r and $\epsilon_{r'}$ the permittivities of the regions *exterior* and *interior* to the surface containing $\mathcal{P}_m$, respectively.

3 Output Modules

In this section we discuss the implementation of some of the SCUFF-STATIC output modules.

3.1 Capacitance matrix

Consider a geometry consisting of N conducting bodies (possibly in the presence of any number of additional dielectric bodies). The capacitance matrix is an $N \times N$ matrix whose m, n entry C_{mn} gives the charge induced on body m when conductor n is maintained at a potential of 1 volt and all other conductors are maintained at zero volts. This is computed in SCUFF-STATIC by performing N separate electrostatic calculations—that is, solving equation (11) for N separate RHS vectors but the same matrix in each case—with the nth RHS vector $\mathbf{v}_n$ corresponding to the case in which the conductor potentials are

$$V_m = (1 \text{ volt}) \cdot \delta_{mn}, \qquad m = \{1, \cdots, N\}.$$

After solving the system for $\boldsymbol{\sigma}$, we compute the total induced charge on body m by simply summing the charges of all panels on that body:

$$C_{mn} = \epsilon_0 \cdot \sum_{p \in \text{panels on } \mathcal{S}_m} A_p \sigma_p$$

where A_p is the panel area.

3.2 Polarizability

The polarizability tensor $\boldsymbol{\alpha}$ measures the dipole moment induced on a body by a spatially-constant external electrostatic field. More specifically, the cartesian components of the dipole moment are related to the cartesian components of the electric field by

$$p_i = \alpha_{ij} E_j.$$

The polarizability is computed in SCUFF-STATIC by solving three separate electrostatics problems—involving constant unit-strength $\mathbf{E}$ fields pointing in each of the three cartesian directions—and computing the resulting dipole moments. Dipole moments $\mathbf{p}$ are computed by summing the charge on each panel times the centroid of the panel:

$$\mathbf{p} = \sum_p A_p \sigma_p \mathbf{x}_p.$$

3.3 C-matrix

The "C-matrix" (not to be confused with the capacitance matrix) is a sort of DC version of the "T-matrix" familiar from full-wave electromagnetic scattering

theory.[4] The rows and columns of the C-matrix are indexed by spherical harmonic indices (ℓm). In brief, the matrix entry $C_{\ell' m', \ell m}$ is the coefficient of the $(\ell' m')$ spherical multipole term in the "scattered" or "outgoing" electrostatic potential due to an object exposed to an "incoming" $(\ell, m)-$spherical multipole field.

Real-valued spherical harmonics

SCUFF-STATIC works in a basis of *real-valued* spherical harmonics $\mathcal{Y}_{\ell m}$. These are defined in terms of the usual complex-valued spherical harmonics $Y_{\ell m}$ by simply replacing the $e^{im\phi}$ factor in Y with a $\cos m\phi$ factor for positive m and a $\sin m\phi$ factor for negative m (and then adjusting the overall normalization such that the new functions are orthonormal). More specifically, we put

$$\mathcal{Y}_{\ell,m} \equiv \begin{cases} \frac{1}{\sqrt{2}}\Big[Y_{\ell,m} + (-1)^m Y_{\ell,-m}\Big], & m > 0 \\ Y_{\ell,m} & m = 0 \\ \frac{1}{i\sqrt{2}}\Big[Y_{\ell,m} - (-1)^m Y_{\ell,-m}\Big], & m < 0. \end{cases} \tag{12}$$

The $\mathcal{Y}$ functions satisfy the orthogonality relation

$$\int \mathcal{Y}_{\ell m}(\theta,\phi)\, \mathcal{Y}_{\ell' m'}(\theta,\phi)\, d\Omega = \delta_{\ell,\ell'}\delta_{m,m'}$$

It is convenient to introduce a single index α that runs over (ℓ, m) tuples according to

$$\alpha(\ell, m) = \ell(\ell+1) + m.$$

[4] Recall that SCUFF-EM includes a code for computing full-wave T-matrices for objects of arbitrary shapes and materials: `http://homerreid.com/scuff-EM/scuff-tmatrix`.

The following table lists the α indices and $\mathcal{Y}$ functions for the first few (ℓ, m) tuples:

α	(ℓ, m)	$\mathcal{Y}_{\ell m}$
0	$(0, 0)$	$+\sqrt{\frac{1}{4\pi}}$
1	$(1, -1)$	$-\sqrt{\frac{3}{4\pi}}\sin\theta\sin\phi$
2	$(1, 0)$	$+\sqrt{\frac{3}{4\pi}}\cos\theta$
3	$(1, +1)$	$-\sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi$
4	$(2, -2)$	$-\sqrt{\frac{15}{16\pi}}\sin^2\theta\sin 2\phi$
5	$(2, -1)$	$-\sqrt{\frac{15}{16\pi}}\cos\theta\sin\theta\sin\phi$
6	$(2, 0)$	$+\sqrt{\frac{5}{16\pi}}(1 + 3\cos 2\theta)$
7	$(2, +1)$	$-\sqrt{\frac{15}{16\pi}}\cos\theta\sin\theta\cos\phi$
8	$(2, +2)$	$+\sqrt{\frac{15}{16\pi}}\sin^2\theta\cos 2\phi$

Definition of C-matrix

The entries of the C-matrix are defined as the coefficients in a spherical-wave expansion of the "outgoing" or "scattered" potential due to a given "incident" or "external" spherical-wave potential. More generally, we consider an object subject to a given external potential $\phi^{\rm ext}(\mathbf{x})$. The total potential is the sum of the external potential plus a "scattered" contribution arising from the induced charge density on the object:

$$\phi(\mathbf{x}) = \phi^{\rm ext}(\mathbf{x}) + \phi^{\rm scat}(\mathbf{x}). \tag{13}$$

To define the C-matrix, we take the external potential to be a unit-strength "incoming" (ℓ, m) spherical wave:

$$\phi^{\rm ext}(\mathbf{x}) = r^{\ell}\mathcal{Y}_{\ell m}(\theta, \phi). \tag{14}$$

Then the "scattered" potential can quite generally be represented as a sum of "outgoing" spherical waves, and the coefficients in this expansion are the elements of the C-matrix:

$$\phi^{\rm scat}(\mathbf{x}) = \sum_{\ell', m'} C_{\ell' m', \ell m} \frac{\mathcal{Y}_{\ell' m'}(\theta, \phi)}{r^{\ell'+1}}. \tag{15}$$

C-matrix elements from charge-density projections

The elements of the C-matrix may be computed from the induced surface charge density $\sigma(\mathbf{x})$ on the surfaces of the objects in a scattering problem. To do so, first note that the "scattered" potential may be obtained from σ in the form of a surface integral:

$$\phi^{\rm scat}(\mathbf{x}) = \int G(\mathbf{x}-\mathbf{x}')\sigma(\mathbf{x}')d\mathbf{x}' \tag{16}$$

where $G(\mathbf{r}) = \frac{1}{4\pi|\mathbf{r}|}$ is the usual electrostatic Green's function. Now insert the spherical-wave expansion of G:

$$= \int \left\{ \sum_{l'm'} \frac{1}{(2l'+1)} \frac{(r')^{\ell'}}{r^{\ell'+1}} \mathcal{Y}_{\ell'm'}(\theta,\phi)\mathcal{Y}_{\ell'm'}(\theta',\phi') \right\} \sigma(\mathbf{x}')d\mathbf{x}' \tag{17}$$

$$= \sum_{l'm'} \Bigg[\underbrace{\frac{1}{(2l'+1)} \int (r')^{\ell'} \mathcal{Y}_{\ell'm'}(\theta',\phi')\sigma(\mathbf{x}')d\mathbf{x}'}_{=C_{\ell'm',\ell m}} \Bigg] \frac{\mathcal{Y}_{\ell'm'}(\theta,\phi)}{r^{\ell'+1}}. \tag{18}$$

Comparing to (15), we have the relation between the C-matrix coefficients and the charge density induced by the incoming $(\ell,m)-$wave potential:

$$C_{\ell'm',\ell m} = \frac{1}{(2l'+1)} \int (r')^{\ell'} \mathcal{Y}_{\ell'm'}(\theta',\phi')\sigma(\mathbf{x}')d\mathbf{x}'. \tag{19}$$

Computation of C-matrix in SCUFF-STATIC

The computation of the C-matrix now proceeds in analogy to the capacitance calculation outlined above:

1. We solve the BEM electrostatics problem (11) with the RHS vector corresponding to an (ℓ,m) external field:

$$\phi^{\rm ext}(\mathbf{x}) = r^{\ell}\mathcal{Y}_{\ell m}(\theta,\phi). \tag{20}$$

2. Then, for each (ℓ',m'), we compute the (ℓ',m') spherical-multipole moment of the induced charge distribution:

$$C_{\ell'm',\ell m} = \frac{1}{2l'+1} \oint d\mathbf{x}\, r^{\ell'} \mathcal{Y}_{\ell'm'}(\hat{\mathbf{x}})\, \sigma(\mathbf{x})$$

   where the surface integral ranges over all surfaces in the problem. We evaluate the integral approximately via a one-point cubature that pretends the integrand is constant over the surface of each panel and equal to its value at the panel centroid:

$$\approx \sum_p A_p \sigma_p |\mathbf{x}_p|^{\ell'} \mathcal{Y}_{\ell'm'}(\hat{\mathbf{x}}_p)$$

where the sum is over all panels on all object surfaces and $\mathbf{x}_p$ is the centroid of panel $\mathcal{P}_p$.

(Note that the C-matrix computed is the C-matrix for the entire geometry including all objects).

Comparison to the usual C-matrix

How do the elements of our C-matrix, defined in terms of real-valued spherical harmonics, compare with the usual definition in terms of the usual complex-valued spherical harmonics? (We will use the notation $\overline{C}_{\ell' m', \ell m}$ to indicate the matrix elements as defined by this usual definition.) In the usual definition, we take the "incident" field to be

$$\phi^{\rm ext}(\mathbf{x}) = r^\ell Y_{\ell m}(\theta, \phi) \tag{21}$$

and then define the $\overline{C}$-matrix entries according to

$$\phi^{\rm scat}(\mathbf{x}) = \sum_{\ell', m'} \overline{C}_{\ell' m', \ell m} \frac{Y_{\ell' m'}(\theta, \phi)}{r^{\ell'+1}}. \tag{22}$$

Here we are using the symbol $\overline{C}$ for the entries of the C-matrix.

To obtain the relation between the $\mathbf{C}$ and $\overline{\mathbf{C}}$ matrices, consider an external field consisting of a superposition of incoming real-valued spherical waves:

$$\phi^{\rm ext} = \sum_{\ell, m} a_{\ell, m} r^\ell \mathcal{Y}_{\ell, m}(\theta, \phi) \tag{23}$$

and write the external field as a superposition of outgoing real-valued spherical waves:

$$\phi^{\rm scat} = \sum_{\ell, m} b_{\ell, m} \frac{\mathcal{Y}_{\ell, m}(\theta, \phi)}{r^{\ell+1}}. \tag{24}$$

Then the $a_{\ell,m}$ and $b_{\ell,m}$ coefficients are related according to

$$\mathbf{b} = \mathbf{C}\mathbf{a} \tag{25}$$

where $\mathbf{a}, \mathbf{b}$ are vectors of a and b coefficients and $\mathbf{C}$ is the C-matrix as defined above with real-valued spherical harmonics.

On the other hand, we could just as easily have expressed the *same* external and scattered fields in terms of complex-valued spherical harmonics,

$$\phi^{\rm ext} = \sum_{\ell, m} \overline{a}_{\ell, m} r^\ell Y_{\ell, m}(\theta, \phi), \qquad \phi^{\rm scat} = \sum_{\ell, m} \overline{b}_{\ell, m} \frac{Y_{\ell, m}(\theta, \phi)}{r^{\ell+1}} \tag{26}$$

in which case the vectors of $\overline{b}$ and $\overline{a}$ coefficients would be related by the conventionally-defined C-matrix,

$$\overline{\mathbf{b}} = \overline{\mathbf{C}}\overline{\mathbf{a}}. \tag{27}$$

Finally, the a and b coefficients may be related to the $\overline{a}$ and $\overline{b}$ coefficients using the definition (12), which reads

$$\mathbf{\Gamma a} = \overline{\mathbf{a}}, \qquad \mathbf{\Gamma b} = \overline{\mathbf{b}}$$

where the elements of the $\mathbf{\Gamma}$ matrix are

$$\Gamma_{\ell m,\ell' m'} = \begin{cases} \frac{\delta_{\ell\ell'}}{\sqrt{2}}\left[\delta_{m,m'} + (-1)^m \delta_{m,-m'}\right], & m' > 0 \\ \delta_{\ell\ell'}\delta_{m0}, & m' = 0 \\ \frac{\delta_{\ell\ell'}}{i\sqrt{2}}\left[\delta_{m,m'} - (-1)^m \delta_{m,-m'}\right], & m' < 0. \end{cases} \tag{28}$$

(Note that $\mathbf{\Gamma}$ is unitary, $\mathbf{\Gamma}^\dagger = \mathbf{\Gamma}^{-1}$.) Using these equations, I can rewrite (25) in the form

$$\mathbf{\Gamma}^\dagger \overline{\mathbf{b}} = \mathbf{C}\mathbf{\Gamma}^\dagger \overline{\mathbf{a}}$$

or

$$\overline{\mathbf{b}} = \mathbf{\Gamma}\mathbf{C}\mathbf{\Gamma}^\dagger \overline{\mathbf{a}}. \tag{29}$$

Comparing (29) to (27) yields the transformation matrix from the real-valued spherical-wave C matrix to the conventionally-normalized $\overline{C}$-matrix:

$$\overline{\mathbf{C}} = \mathbf{\Gamma}\mathbf{C}\mathbf{\Gamma}^\dagger. \tag{30}$$