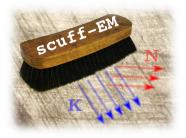


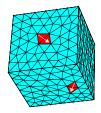
Surface Integral Equations and the Boundary Element Method

> Homer Reid 18.369 Guest Lecture 3/23/2012





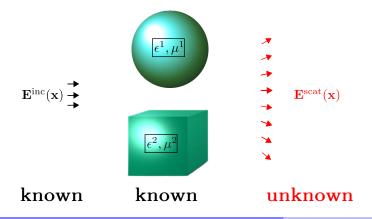








We have some known **incident field** (such as a plane wave), scattering from some known **geometry** (including objects of known shapes and materials) and we want to know the scattered fields. (Note: all quantities  $\sim e^{-i\omega t}$ .)

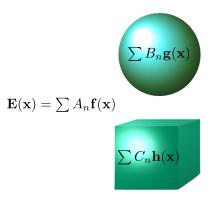




# Methods for Solving EM Scattering Problems, 1

Expansions in special functions

Write the fields inside and outside the scatterer as expansions in sets of known Maxwell solutions (in some convenient coordinate system) and match coefficients.



## Advantages:

• Exploits known Maxwell solutions  $\implies$  efficient

## **Disadvantages:**

 Only works for a small number of geometries → not general.

**One Sphere**: "Mie scattering"

 $\mathbf{f}(\mathbf{x}) \sim j_l(r) Y_{lm}(\theta, \phi)$ 

Planar Slab: "Fresnel Coefficients"

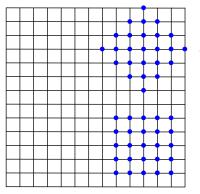
 $\mathbf{f}(\mathbf{x}) \sim e^{i\mathbf{k}\cdot\mathbf{x}}$ 



# Methods for Solving EM Scattering Problems, 2

## Finite-Difference Method

- Discretize the geometry onto a grid (each grid point can have different  $\epsilon,\mu)$
- Write Maxwell's equations using finite-difference approximations to derivatives
- Solve sparse linear system for the E-field values at grid points



$$\begin{bmatrix} \nabla \times \nabla \times -k^2 \end{bmatrix} \mathbf{E} = -i\omega \mathbf{J} \Longrightarrow \begin{pmatrix} \mathbf{M} \end{bmatrix} \begin{pmatrix} \mathbf{E}_1 \\ \vdots \\ \mathbf{E}_n \end{pmatrix} = i\omega \begin{pmatrix} \mathbf{J}_1 \\ \vdots \\ \mathbf{J}_n \end{pmatrix}$$

## Advantages:

- Allows different  $\epsilon, \mu$  at each grid point  $\longrightarrow$  general
- Relatively easy to implement

## **Disadvantages:**

- Does not make use of known Maxwell solutions  $\longrightarrow$  not the most efficient method
- If we need to evaluate the scattered fields far from the scattering objects, we have to discretize the entire space between the objects and the evaluation point. → Seems wasteful.

# Methods for Solving EM Scattering Problems, 3 Surface-Integral-Equation (SIE) Method

- First compute the surface current distribution  $\mathbf{K}(\mathbf{x})$  induced by the incident field
- Then compute the scattered fields using  $\mathbf{K}(\mathbf{x})$  and known Maxwell solutions:

$$\mathbf{E}^{\mathsf{scat}}(\mathbf{x}) = \oint_{S} \mathbf{G}(\mathbf{x} - \mathbf{x}') \mathbf{K}(\mathbf{x}') d\mathbf{x}' \quad \text{ where } \mathbf{G} \text{ is the solution to } \quad \left[ \nabla \times \nabla \times \ -k^2 \right] \mathbf{G}(\mathbf{r}) = -i\omega \mathbf{1}\delta(\mathbf{r});$$

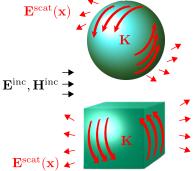
G (the "dyadic Green's function") is known in closed form

## **Advantages:**

- Exploits known Maxwell solutions  $\implies$  efficient
- Allows scatterers of arbitrary shapes and arbitrary (homogeneous) materials  $\implies$  general
- Unknown quantities confined to object surfaces, not everywhere in space  $\implies$  not wasteful

## **Disadvantages:**

- Difficult to implement
- Restricted to homogeneous scatterers, i.e. piecewise-constant  $\epsilon, \mu$





# SIE Formulation of Scattering Problems

Consider a perfectly electrically conducting (PEC) scatterer in vacuum.

The incident field induces a surface electric current density  $\mathbf{K}(\mathbf{x})$  on the object surface.

Surface current density  $\mathbf{K}$ : units of  $\frac{\text{current}}{\text{length}}$ 

 $\underbrace{\mathbf{J}(\mathbf{x}_{\parallel}, z)}_{\text{volume current}} = \underbrace{\mathbf{K}(\mathbf{x}_{\parallel})}_{\text{surface current}} \cdot \delta(z)$ 

Once we know  $\mathbf{K}(\mathbf{x})$ , we can compute the scattered  $\mathbf{E}$ -field anywhere we like:

$$\mathbf{E}^{\mathsf{scat}}(\mathbf{x}) = \oint_{\mathcal{S}} \mathbf{G}(\mathbf{x} - \mathbf{x}') \mathbf{K}(\mathbf{x}') d\mathbf{x}'$$

$$G_{ij}(\mathbf{r}) = \frac{e^{ikr}}{4\pi k^2 r^3} \left\{ \left[ 1 - ikr + (ikr)^3 \right] \delta_{ij} + \left[ -3 + 3ikr - (ikr)^2 \right] \frac{\mathbf{r}_i \mathbf{r}_j}{r^2} \right\} \qquad \left( r = |\mathbf{r}|, \quad k = \frac{\omega}{c} \right)$$

We determine  $\mathbf{K}(\mathbf{x})$  by requiring that the total tangential E-field vanish at the object surface:

$$\left[\mathbf{E}^{\mathsf{inc}}(\mathbf{x}) + \mathbf{E}^{\mathsf{scat}}(\mathbf{x})\right]_{\parallel} = 0 \qquad \Longrightarrow \qquad$$

(for points x on object surfaces)

$$\oint_{\mathcal{S}} \mathbf{G}_{\parallel}(\mathbf{x},\mathbf{x}') \mathbf{K}(\mathbf{x}') d\mathbf{x}' = -\mathbf{E}_{\parallel}^{\text{inc}}(\mathbf{x})$$

"electric field integral equation" (EFIE)

The EFIE is an integral equation for  $\mathbf{K}(\mathbf{x})$  in terms of  $\mathbf{E}^{\mathsf{inc}}$ .



# Numerical Solution of SIEs

The boundary element method (BEM)

Given 
$$\mathbf{E}^{\text{inc}}(\mathbf{x})$$
, want to find  $\mathbf{K}(\mathbf{x})$  that solves the EFIE: 
$$\oint_{\mathcal{S}} \mathbf{G}_{\parallel}(\mathbf{x}, \mathbf{x}') \mathbf{K}(\mathbf{x}') d\mathbf{x}' = -\mathbf{E}_{\parallel}^{\text{inc}}(\mathbf{x})$$

Idea: (1) expand  $\mathbf{K}(\mathbf{x})$  in some convenient set of N basis functions  $\Longrightarrow N$  unknown coefficients

$$\mathbf{K}(\mathbf{x}) = \sum_{n=1}^{N} k_n \mathbf{f}_n(\mathbf{x}), \qquad \left\{ \mathbf{f}_n(\mathbf{x}) \right\} = \begin{pmatrix} \text{tangential vector-valued basis functions} \\ \text{defined on the object surface} \end{pmatrix}$$

Idea: (2) test (inner-product) the EFIE with each basis function  $\implies N$  equations

$$\left\langle \mathbf{f}_{m}, \oint \mathbf{G} \underbrace{\mathbf{K}}_{\sum k_{n} \mathbf{f}_{n}} dA \right\rangle = -\left\langle \mathbf{f}_{m}, \mathbf{E}^{\mathsf{inc}} \right\rangle \qquad \Longrightarrow \qquad \left( \begin{array}{c} \mathbf{M} \end{array} \right) \left( \begin{array}{c} k_{1} \\ \vdots \\ k_{N} \end{array} \right) = \left( \begin{array}{c} v_{1} \\ \vdots \\ v_{N} \end{array} \right)$$

 $N \times N$  linear system ("BEM system")

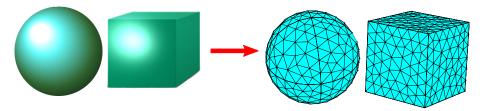
Matrix elements:  $M_{mn} = \left\langle \mathbf{f}_m \middle| \mathbf{G} \middle| \mathbf{f}_n \right\rangle$  RHS vector:  $v_m = -\left\langle \mathbf{f}_m \middle| \mathbf{E}^{\mathsf{inc}} \right\rangle$ 



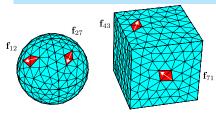
# Basis functions for SIE/BEM solvers

One choice for compact 3D objects: "RWG basis functions" ·

## Begin by discretizing ("meshing") object surfaces into triangles:



### Associate one basis function with each internal edge:



- These are "RWG basis functions" (named for their inventors: Rao, Wilton, Glisson)
- # of basis functions  $N \propto \#$  of triangles
- As we refine the discretization (shrink the triangles), the discretization errors decrease, but the cost of solving the linear system grows like  $N^3$



# Steps in a BEM Scattering Calculation

For a compact 3D scattering problem using RWG basis functions

- 1. Discretize object surfaces into triangles.
  - A well-studied problem; high-quality free software packages are available.
- 2. Analyze the surface mesh and assign one basis function  $\mathbf{f}_n(\mathbf{x})$  to each interior edge.
  - Some minor computational work; not too challenging.
- 3. Most difficult step: Assemble the BEM matrix  ${\bf M}$  and RHS vector  ${\bf v}.$

$$M_{mn} = \left\langle \mathbf{f}_m \middle| \mathbf{G} \middle| \mathbf{f}_n \right\rangle, \qquad v_m = -\left\langle \mathbf{f}_m \middle| \mathbf{E}^{\mathsf{inc}} \right\rangle$$

- 4. Solve the linear system  $M\mathbf{k} = \mathbf{v}$  for the surface-current expansion coefficients  $\{k_n\}$ .
  - For  $N \lesssim 10,000$ , use standard linear algebra software (LAPACK).
- 5. Use the surface current density  $\mathbf{K}(\mathbf{x}) = \sum k_n \mathbf{f}_n(\mathbf{x})$  to compute the scattered fields.

$$\boxed{\mathbf{E}^{\mathsf{scat}}(\mathbf{x}) = \sum_{n} k_n \int \mathbf{G}^{\mathsf{EE}}(\mathbf{x}, \mathbf{x}') \mathbf{f}_n(\mathbf{x}') d\mathbf{x}', \qquad \mathbf{H}^{\mathsf{scat}}(\mathbf{x}) = \sum_{n} k_n \int \mathbf{G}^{\mathsf{ME}}(\mathbf{x}, \mathbf{x}') \mathbf{f}_n(\mathbf{x}') d\mathbf{x}',}$$

where  $\mathbf{G}^{\mathsf{EE}}$  is what we called "G" before and  $\mathbf{G}^{\mathsf{ME}}\sim \nabla\times\mathbf{G}^{\mathsf{EE}}.$ 

Consider a scattering geometry with surfaces discretized into  $N \sim 10,000$  triangles.

- 1. We have  $N^2 = 100$  million matrix elements.
- 2. Each matrix element involves a 4 dimensional integral (surface integrals over two triangles) that must be evaluated numerically.
- 3. A sizeable fraction of these are singular integrals.

$$\frac{M_{mn} = \left\langle \mathbf{f}_{m} \middle| \mathbf{G} \middle| \mathbf{f}_{n} \right\rangle}{M_{mn} = \left\langle \begin{array}{cccc} M_{11} & M_{12} & M_{13} & \cdots & M_{1N} \\ M_{21} & M_{22} & M_{23} & \cdots & M_{2N} \\ M_{31} & M_{32} & M_{33} & \cdots & M_{3N} \\ \vdots & \vdots & \ddots & \vdots \\ M_{N1} & M_{N2} & M_{N3} & \cdots & M_{NN} \end{array}}\right)_{10,000} \\
\int_{T} d\mathbf{x} \int_{T'} d\mathbf{x}' h(\mathbf{x}, \mathbf{x}') g(|\mathbf{x} - \mathbf{x}'|) \\ T & T' & T \\ T' & T' \\ T' & T'$$



## research

#### Codes

Casimir Electromagnetic Scattering Quantum Chemistry

Numerical Libraries

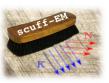
#### Talks

Thesis Defense Zeta Function Intro Ouantum Chem IFC Poster 12/05 CNTFET Modeling

#### Memos

PhD Thesis BEM Tutorial ID Waveguide Tapering Debye-Huckel Boundary Conditions Second-Order Self Energy Diagrams Modeling Nanotubes

Publications



### SCUFF-EM: Free, open-source software for boundary-element analysis of problems in computational physics and engineering

SCUFF-EM is a free, open-source software package for analysis of electromagnetic scattering problems using the boundary-element method (BEM). (The BEM is also known as the "method of moments.")

The sCUFF-EM suite consists of two components: a *core library* that implements the essential algorithms of the boundary-element method, and a set of *application programs* built atop the core library for solving specific problems in various fields of physics and engineering.

The core library, LIBSCUFF, is written in c++ but may also be accessed from PYTHON and MATLAB. Extensive documentation of the programming interfaces is available from the links below.

The application programs, implemented as console-based command-line utilities, include tools for (10) general electromagnetic scattering of arbitrary includent fields from compact or periodically extended scatterers; (2) computation of Casimir forces and Casimir-Folder potentials in complexgeneratic and material configurations; and (3) modeling of RF and microwet devices, includingcomputation of multiport network parameters and radiated fields for antennas, lumped elements,and other RF devices.

The entire SCUFF-EM suite is free software distributed under the GNU GPL.

SCUFF-EM stands for Surface CUrrent/Field Formulation of ElectroMagnetism. This is a reference to the underlying solution methodology used by SCUFF-FM and other BFM solvers in which we solve

#### SCUFF-EM

#### Installation

Core Library

- Library Reference
- <u>c++ interface</u>
- PYTHON interface
- MATLAB interface

#### Applications

- Electromagnetic Scattering
   o <u>SCUFF-SCATTER</u>
   o SCUFF-SCATTER-PERIODIC
- Casimir Physics

   SCUFF-CAS3D
  - o SCUEE-CAS2D
  - SCUFF-CASPOL
- RF/Microwave Engineering
   o SCUFF-RF

Referen



# SIE/BEM Techniques for Non-PEC Geometries

For non-PEC geometries we must introduce effective magnetic surface currents

For PEC scatterers, the SIE/BEM procedure reflects a physical reality: the currents induced by the incident field are confined to the object surface.

For general (non-PEC) scatterers, this is no longer true: the incident field induces currents throughout the volume of the scatterer.

Two		
options:		

- 1. Volume integral equation: Write an integral equation for the volume electric current distribution  $J(\mathbf{x})$  throughout the bulk of the scatterer.
- 2. Surface integral equation: Write an integral equation for effective electric and magnetic surface currents  $\mathbf{K}(\mathbf{x}), \mathbf{N}(\mathbf{x})$  on the surface of the scatterer.

	PEC	Non-PEC
Physics	Surface electric current ${f K}$	Volume electric current ${f J}$
Mathematics	Surface electric current ${f K}$	Surface electric and magnetic currents $\mathbf{K}, \mathbf{N}$







## Effective Surface Currents for non-PEC Geometries

## The Stratton-Chu equations

Recall Green's theorem: For a scalar field  $\phi$  satisfying Laplace, knowledge of  $\phi$  (or  $\frac{\partial \phi}{\partial \hat{n}}$ ) on the boundary  $\partial \Omega$  of a closed source-free region  $\Omega$  suffices to recover  $\phi$  everywhere in the interior.



The Stratton-Chu equations generalize Green's theorem to the case of vector fields satifying Maxwell: knowledge of tangential  $\mathbf{E}$ ,  $\mathbf{H}$  on  $\partial\Omega$  suffices to recover  $\mathbf{E}$  and  $\mathbf{H}$  throughout  $\Omega$ .

$$\begin{split} \mathbf{E}(\mathbf{x}) &= \oint_{\partial \Omega} \left\{ \mathbf{G}^{\mathsf{EE}}(\mathbf{x}, \mathbf{x}') \Big[ \hat{\mathbf{n}} \times \mathbf{H}(\mathbf{x}') \Big] + \mathbf{G}^{\mathsf{EM}}(\mathbf{x}, \mathbf{x}') \Big[ - \hat{\mathbf{n}} \times \mathbf{E}(\mathbf{x}') \Big] \right\} dA \\ \mathbf{H}(\mathbf{x}) &= \oint_{\partial \Omega} \left\{ \mathbf{G}^{\mathsf{ME}}(\mathbf{x}, \mathbf{x}') \Big[ \hat{\mathbf{n}} \times \mathbf{H}(\mathbf{x}') \Big] + \mathbf{G}^{\mathsf{MM}}(\mathbf{x}, \mathbf{x}') \Big[ - \hat{\mathbf{n}} \times \mathbf{E}(\mathbf{x}') \Big] \right\} dA \end{split}$$

The source quantities that enter the Stratton-Chu equations are  $\hat{\mathbf{n}} \times \mathbf{H}$  and  $-\hat{\mathbf{n}} \times \mathbf{E}$ . Think of these as effective surface currents:

$$\mathbf{K}^{eff}(\mathbf{x}) \equiv \mathbf{\hat{n}} \times \mathbf{H}, \qquad \mathbf{N}^{eff}(\mathbf{x}) \equiv -\mathbf{\hat{n}} \times \mathbf{E}.$$





# BEM Formulation for non-PEC Scatterers

Generalizing the EFIE

Fields inside and outside the scatterer:

$$\begin{bmatrix} \mathbf{E}^{in}(\mathbf{x}) \\ \mathbf{H}^{in}(\mathbf{x}) \end{bmatrix} = -\oint_{\partial\Omega} \begin{bmatrix} \mathbf{G}^{in}(\mathbf{x}, \mathbf{x}') \end{bmatrix} \begin{bmatrix} \mathbf{K}(\mathbf{x}') \\ \mathbf{N}(\mathbf{x}') \end{bmatrix} d\mathbf{x}'$$

$$\begin{bmatrix} \mathbf{E}^{\mathsf{out}}(\mathbf{x}) \\ \mathbf{H}^{\mathsf{out}}(\mathbf{x}) \end{bmatrix} = + \oint_{\partial\Omega} \begin{bmatrix} \mathbf{G}^{\mathsf{out}}(\mathbf{x}, \mathbf{x}') \end{bmatrix} \begin{bmatrix} \mathbf{K}(\mathbf{x}') \\ \mathbf{N}(\mathbf{x}') \end{bmatrix} d\mathbf{x}' + \begin{bmatrix} \mathbf{E}^{\mathsf{inc}}(\mathbf{x}) \\ \mathbf{H}^{\mathsf{inc}}(\mathbf{x}) \end{bmatrix}$$

**Match tangential fields** at the scatterer surface (for points  $\mathbf{x} \in \partial \Omega$ ):

 $\mathbf{E}^{\text{in}}_{\parallel}(\mathbf{x}) \quad = \mathbf{E}^{\text{out}}_{\parallel}(\mathbf{x})$  $\left| \oint_{\partial \Theta} \left[ \mathbf{G}^{\mathsf{out}} + \mathbf{G}^{\mathsf{in}} \right]_{\parallel} \left[ \begin{array}{c} \mathbf{K}(\mathbf{x}') \\ \mathbf{N}(\mathbf{x}') \end{array} \right] d\mathbf{x}' = - \left[ \begin{array}{c} \mathbf{E}^{\mathsf{inc}}(\mathbf{x}) \\ \mathbf{H}^{\mathsf{inc}}(\mathbf{x}) \end{array} \right]_{\parallel} \right]$  $\implies$  $\mathbf{H}_{\parallel}^{\text{in}}(\mathbf{x}) = \mathbf{H}_{\parallel}^{\text{out}}(\mathbf{x})$ 

Integral equation for  $\mathbf{K}, \mathbf{N}$  in terms of  $\mathbf{E}^{\text{inc}}, \mathbf{H}^{\text{inc}}$ 

**Discretize** by expanding  $K(\mathbf{x}) = \sum k_n \mathbf{f}_n(\mathbf{x}), \qquad N(\mathbf{x}) = \sum n_n \mathbf{f}_n(\mathbf{x})$ :

$$\left(\begin{array}{c} \mathbf{M} \end{array}\right) \left(\begin{array}{c} k_n \\ n_n \end{array}\right) = \left(\begin{array}{c} v_n^{\mathsf{E}} \\ v_n^{\mathsf{H}} \end{array}\right)$$

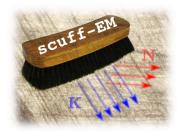
("PMCHW Formulation")

 $\implies 2N \times 2N$  linear system for the expansion coefficients  $\{k_n, n_n\}$ 



# SCUFF-EM: An open-source BEM code suite

Surface-Current / Field Formulation of ElectroMagnetism



## http://homerreid.com/scuff-EM

## Features currently available:

- Scattering from compact 3D objects of arbitrary shapes
- Arbitrary user-specified frequency-dependent  $\epsilon, \mu$  (isotropic, linear, piecewise constant)
- Linux/Athena command-line interface to scattering code
- C++ interface to scattering code
- Application modules: Casimir forces, RF device modeling

## Features coming soon:

- Python / Matlab interfaces to scattering codes
- Scattering from periodic geometries

# Solving scattering problems with SCUFF-EM

Scattering of a gaussian laser beam from a silver nanotip

