Efficient Effective Media Calculations Applied to the Sparse Matrix/Canonical Grid Method in 3-D

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Presentation Outline

I. Introduction and Motivation

II. Effective Media
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   2. Previous results

III. 3-D Sparse Matrix/Canonical Grid (SMCG) Method
   1. Method overview
   2. Method parameters – $\gamma$, $r_d$, and $N_g$
   3. Dyadic Green’s function expansion
   4. FFT assisted fast multiply

IV. Results

V. Conclusion
Introduction – Motivation

Mixtures and Compounds – Homogeneous substances containing discrete inclusions

- Electrically small discrete scatterers
- Random distribution
- Nontenuous, densely packed
- Examples: snow, soil, composite materials, RAMs, optical filters
- Many media not fully characterized by spherical characteristics

Note: Independent scattering assumption no longer valid
Effective Media Approach

Effective Permittivity

- Permittivity at which homogeneous medium responds to electromagnetic excitation in the same manner as a random medium
- Response of homogeneous medium dependent upon size, shape, and $\varepsilon_{eff}$
- Scattered coherent field from random media in a test volume is compared to those from a homogeneous volume with the same size and shape
Random Media Characterization

\[ \varepsilon_{eff} \rightarrow \varepsilon_{eff}(ka, \text{shape}, \text{contrast}, f_v, \text{Arrangement}, \ldots) \]

Various limiting cases result in tractable analytical theories, but many real-world applications cannot be modeled by these limiting cases.
Monte Carlo Simulation Parameters

* Assume $\epsilon_{eff}$ is purely real

Find $\epsilon_{eff}$ which minimizes:

$$\text{error} = \sum_{j=1}^{N_a} |(\sigma_{mie,j}(\epsilon_{eff})) - (\sigma_{ran,j})|$$

where $N_a$ is the number of angles

For this case –

$$f_v = 0.25$$

$$e = 1.0 \text{ (sphere)} \text{ and } 1.8$$

$$ka = 0.2 \text{ and }$$

$$\epsilon_p = 3.2 + 0.0i$$
Previous Results

Table 1. Results. For all cases, $ka = 0.2$ and $\varepsilon_p = 3.2 + 0.0 \dot{\varepsilon}$.

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SMCG and SMCG-Multilevel

Sparse Matrix Canonical Grid

( Tsang, et al. 1993 )

- Strong interactions calculated and stored or calculated each time
- Weak interactions expanded around canonical gridpoints

Examples

- Multilayer grid for 2-D scattering from rough surfaces ( Li, et al., 2000 )
- Scattering from collections of dielectric cylinders ( Chan and Tsang, 1995 )
3-D Sparse Matrix Canonical Grid Method (SMCG)

3-D SMCG Method

1. Construct a cubic mesh in the region of interest
2. Decide on a strong interaction radius, $r_d$
   - Construct strong interaction matrix for particles inside $r_d$
   - Construct weak interaction matrix for particles outside than $r_d$
3. Performance increases due to structure inherent in separated interaction matrices
SMCG General Formulation

Many-Body Volume Integral Equation

\[ \bar{E}(\tau) = \bar{E}_{\text{inc}}(\tau) + \frac{k^2}{\epsilon} \sum_{j=1}^{N} \int_{V_j} dV_j' \ (\epsilon(\tau_j') - \epsilon) \ \bar{G}(\tau, \tau_j') \cdot \bar{E}(\tau_j') \]

where

\( N \) = number of particles

\( V_j \) = volume of scatterer \( j \)

\( k \) = wavenumber of the background medium

\( \epsilon \) = permittivity of the background medium

\( \epsilon(\tau_j') \) = permittivity inside the \( j^{th} \) scatterer

\( \bar{G}(\tau, \tau_j') \) = background dyadic Green’s function
Scattering Solution

II Solve for $\overline{E}(\overline{r})$ by Method of Moments

- Basis Functions

$$\overline{E}(\overline{r}_j') = \sum_{\alpha=1}^{N_b} c_{j\alpha} \overline{f}_{j\alpha}(\overline{r}_j')$$

where

$$\overline{f}_{j\alpha}(\overline{r}_j') = \text{basis functions for } j^{th} \text{ particle}$$

$$c_{j\alpha} = \text{expansion amplitudes}$$

- Substituting:

$$\left[ \sum_{\beta=1}^{N_b} c_{i\beta} \overline{f}_{i\beta}(\overline{r}_i') \right] = \overline{E}_{inc}(\overline{r}_i') + \frac{k_v^2}{\epsilon} \sum_{j=1}^{N} \int_{V_j'} dV_j' \left( \epsilon(\overline{r}_j') - \epsilon \right) \overline{G}(\overline{r}_i', \overline{r}_j') \cdot \left[ \sum_{\alpha=1}^{N_b} c_{j\alpha} \overline{f}_{j\alpha}(\overline{r}_j') \right]$$
Scattering Solution (cont.)

Test function

\[
\int_{V_i'} dV' \overline{f}_{i\beta}(\overline{r}'_i) \cdot \left\{ \sum_{\beta=1}^{N_b} c_{i\beta} \overline{f}_{i\beta}(\overline{r}'_i) \right\} = \overline{E}_{inc}(\overline{r}'_i) + \frac{k^2}{\varepsilon} \sum_{j=1}^{N} \int_{V_j'} dV' (\varepsilon(\overline{r}'_j) - \varepsilon) \overline{G}(\overline{r}'_i, \overline{r}'_j) \cdot \left\{ \sum_{\alpha=1}^{N_b} c_{j\alpha} \overline{f}_{j\alpha}(\overline{r}'_j) \right\}
\]

Leads to:

\[c_{i\beta} = \int_{V_i'} dV' \overline{f}_{i\beta}(\overline{r}'_i) \cdot \overline{E}_{inc}(\overline{r}'_i) + c_{j\alpha} \sum_{j=1}^{N} \sum_{\alpha=1}^{N_b} z_{ij,\alpha\beta},\]

where

\[z_{ij,\alpha\beta} = B_{j\alpha} \int_{V_i'} dV' \int_{V_j'} dV' \overline{f}_{i\beta}(\overline{r}'_i) \cdot \overline{G}(\overline{r}'_i, \overline{r}'_j) \cdot \overline{f}_{j\alpha}(\overline{r}'_j),\]

with

\[B_{j\alpha} = \frac{k^2}{\varepsilon} (\varepsilon(\overline{r}'_j) - \varepsilon) \quad \text{and} \quad (B_{j\alpha} z_{ij,\alpha\beta})|_{i=j,\alpha=\beta} = C_{i\beta},\]
Full MoM Solution

Matrix Equation

\[ \mathbf{Z} \cdot \mathbf{x} = \mathbf{b} \]

where

\[ \mathbf{x} = [\{c_{11}, c_{12}, \ldots, c_{1N_b}\}, \ldots, \{c_{N1}, c_{N2}, \ldots, c_{NN_b}\}]^T, \]

\[ \mathbf{Z}_{ij} = \begin{cases} \begin{bmatrix} z_{i,j,11} & z_{i,j,12} & \cdots & z_{i,j,1N_b} \\ z_{i,j,21} & z_{i,j,22} & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ z_{i,j,N_b1} & \cdots & z_{i,j,N_bN_b} \end{bmatrix} & i \neq j, \\ \begin{bmatrix} (1 - C_{i1}) & 0 & \cdots & 0 \\ 0 & (1 - C_{i2}) & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & (1 - C_{iN_b}) \end{bmatrix} & i = j, \end{cases} \]

\[ \mathbf{b} = \begin{bmatrix} \int_{V_1} dV_1' \mathbf{f}_{11}(\mathbf{r}_1') \cdot \mathbf{E}_{inc}(\mathbf{r}_1') \\ \int_{V_1} dV_1' \mathbf{f}_{12}(\mathbf{r}_1') \cdot \mathbf{E}_{inc}(\mathbf{r}_1') \\ \vdots \\ \int_{V_1} dV_1' \mathbf{f}_{1N_b}(\mathbf{r}_1') \cdot \mathbf{E}_{inc}(\mathbf{r}_1') \end{bmatrix}. \]
Interaction Matrix $\bar{Z}$

Small Spheroid Assumption

$$\int_{V_i'} dV_i' \sim v_i = \frac{4}{3} \pi a_i^2 c_i \quad \text{and} \quad \epsilon(\bar{r}_j') \sim \epsilon_j$$

Then $z_{ij,\alpha\beta}$ becomes

$$z_{ij,\alpha\beta} = B_{j\alpha} \int_{V_i'} dV_i' \int_{V_j'} dV_j' \bar{f}_{i\beta}(\bar{r}_i') \cdot \bar{G}(\bar{r}_i', \bar{r}_j') \cdot \bar{f}_{j\alpha}(\bar{r}_j')$$

$$= B_{j\alpha} v_i v_j \bar{f}_{i\beta} \cdot \bar{G}(\bar{r}_i', \bar{r}_j') \cdot \bar{f}_{j\alpha}$$

where $\bar{f}_{i\beta}$ and $\bar{f}_{j\alpha}$ depend only upon the distance to the centers of the particle
Interaction Matrix $\overline{Z}$ (cont.)

Now $\overline{Z}_{ij}$ becomes

$$\overline{Z}_{ij} = \overline{f}_i \cdot \overline{G}(\overline{r}_i', \overline{r}_j') \cdot \overline{f}_j$$

where

$$\overline{f}_i = \begin{bmatrix} f_{i1,x} & f_{i1,y} & f_{i1,z} \\ \vdots & \vdots & \vdots \\ f_{iN_b,x} & f_{iN_b,y} & f_{iN_b,z} \end{bmatrix}, \quad \overline{G}(\overline{r}_i', \overline{r}_j') = \begin{bmatrix} (k^2 + \frac{\partial^2}{\partial x^2})\hat{x}\hat{x} & (\frac{\partial}{\partial x})\hat{x}\hat{y} & (\frac{\partial}{\partial x})\hat{x}\hat{z} \\ (\frac{\partial}{\partial y})\hat{x}\hat{y} & (k^2 + \frac{\partial^2}{\partial y^2})\hat{y}\hat{y} & (\frac{\partial}{\partial y})\hat{y}\hat{z} \\ (\frac{\partial}{\partial z})\hat{x}\hat{z} & (\frac{\partial}{\partial z})\hat{y}\hat{z} & (k^2 + \frac{\partial^2}{\partial z^2})\hat{z}\hat{z} \end{bmatrix} \frac{g(x, y, z)}{k^2}$$

and

$$\overline{f}_j = \overline{f}_i^T \text{ if } i = j$$

And now we express $\overline{Z}$ as

$$\overline{Z} = \overline{f} \cdot \overline{G}(\mathcal{R}) \cdot \overline{f}^T,$$
Here \( N_b = 3 \), and particles \( i = 1, 2, 3 \) are shown. 
Note: Row position is determined by particle index. 
Note: Column position is determined by associated gridpoint.
Decompositions

Decide neighborhood distance \( r_d \)

Decompose \( \mathcal{R} \)

\[
\mathcal{R} \rightarrow \begin{cases} 
\mathcal{R}_s & \forall \mathcal{R} \leq r_d \\
\mathcal{R}_w & \forall \mathcal{R} > r_d
\end{cases} \quad \mathcal{R}_s \cup \mathcal{R}_w = \mathcal{R}
\]

Now decompose \( \overline{G}(\mathcal{R}) \)

\[
\overline{G}(\mathcal{R}) = \overline{G}(\mathcal{R}_s) + \overline{G}^{eg}(\mathcal{R}_w),
\]

and finally \( \overline{Z} \)

\[
\overline{Z} = \overline{Z}_s + \overline{Z}_w = \overline{f} \cdot \overline{G}(\mathcal{R}_s) \cdot \overline{f}^\text{T} + \overline{f} \cdot \overline{G}^{eg}(\mathcal{R}_w) \cdot \overline{f}^\text{T}
\]
We have

\[(\overline{Z}^s + \overline{Z}^w) \cdot \overline{x} = \overline{b}\]

- Use an iterative solver such as *bicgstab* to solve. These CG solvers require only the matrix vector product $\overline{Z} \cdot \overline{x}$

  - $\overline{Z}^s \cdot \overline{x}$ is a sparse multiplication ($O(N)$)

  - $\overline{Z}^w \cdot \overline{x}$ can be computed quickly ($O(N\log(N))$) by exploiting the structure inherent in $\overline{G}^{eg}(\mathcal{R}_w)$
\( \gamma^{th} \) Order Taylor Series Expansion of \( \overline{G}^{eg}(R_w) \)

If particles \( i \) and \( j \) are associated with gridpoints \( g^{l_{imi}} \) and \( g^{l_{jmj}} \) located at \( \overline{r}_{g}^{l_{imi}} \) and \( \overline{r}_{g}^{l_{jmj}} \) respectively, then

\[
\overline{G}^{eg}_{ij}(R_w) = \sum_{\gamma=0}^{\infty} \frac{1}{\gamma!} \left( \Delta x_{ij} \frac{\partial}{\partial x} + \Delta y_{ij} \frac{\partial}{\partial y} + \Delta z_{ij} \frac{\partial}{\partial z} \right)^\gamma \overline{G}(\overline{r}_{g}^{l_{imi}}, \overline{r}_{g}^{l_{jmj}})
\]

or via the trinomial theorem as

\[
\overline{G}^{eg}_{ij}(R_w) = \sum_{\gamma=0}^{\infty} \sum_{\gamma_x+\gamma_y+\gamma_z=\gamma} \left( \frac{1}{\gamma_x! \gamma_y! \gamma_z!} \right) \left( \Delta x_{ij} \right)^{\gamma_x} \left( \Delta y_{ij} \right)^{\gamma_y} \left( \Delta z_{ij} \right)^{\gamma_z} \frac{\partial^{\gamma_x}}{\partial x^{\gamma_x}} \frac{\partial^{\gamma_y}}{\partial y^{\gamma_y}} \frac{\partial^{\gamma_z}}{\partial z^{\gamma_z}} \overline{G}(\overline{r}_{g}^{l_{imi}}, \overline{r}_{g}^{l_{jmj}})
\]

where

\[
\Delta \xi_{ij} = \Delta \xi_i - \Delta \xi_j
\]

\[
= (\overline{r}_{i, \xi} - \overline{r}_{g, \xi}^{l_{imi}}) - (\overline{r}_{j, \xi} - \overline{r}_{g, \xi}^{l_{jmj}})
\]

for \( \xi \Rightarrow x, y, \) or \( z \)
Taylor Expansion (cont.)

Separate particle dependant quantities

\[ \bar{f}_{\gamma x\gamma y\gamma z} \equiv \left( \prod_{\xi=x,y,z} (\Delta \xi)^{\gamma \xi} \right) \bar{f}_i, \quad \forall \ i = 1..N. \]

and gridpoint dependant quantities

\[ \bar{G}_{\gamma x\gamma y\gamma z} \equiv \left( \frac{\gamma!}{\gamma_x!\gamma_y!\gamma_z!} \right) \frac{\partial^{\gamma x}}{\partial x^{\gamma x}} \frac{\partial^{\gamma y}}{\partial y^{\gamma y}} \frac{\partial^{\gamma z}}{\partial z^{\gamma z}} \bar{G}(\bar{r}^{\Delta \Delta m \Delta n}) \]
Taylor Expansion (cont.)

Now we can express $\overline{Z}^w$ as

\[
\overline{Z}^w = \overline{f} \cdot \overline{G}^z(\mathcal{R}_w) \cdot \overline{f}^T
\]

\[
= \sum_{\gamma=0}^{\infty} \sum_{\gamma_x+\gamma_y+\gamma_z=\gamma} \overline{Z}^w_{\gamma_x\gamma_y\gamma_z}
\]

where

\[
\overline{Z}^w_{\gamma_x\gamma_y\gamma_z} = \sum \sum \sum (-1)^{\gamma_{x_2}+\gamma_{y_2}+\gamma_{z_2}} \left( \begin{array}{c}
\gamma_{x_2} \\
\gamma_{y_2} \\
\gamma_{z_2}
\end{array} \right) \left( \begin{array}{c}
\gamma_x \\
\gamma_y \\
\gamma_z
\end{array} \right) \overline{f} \gamma_{x_1} \gamma_{y_1} \gamma_{z_1} \overline{G} \gamma_{x_2} \gamma_{y_2} \gamma_{z_2} \overline{f}^T
\]
Example

For example, for $\gamma = 2$

\[
(\overline{Z}^s + \overline{Z}^w) \cdot \overline{x} = \overline{b}
\]

\[
\left( \overline{f} \cdot \overline{G(R_s)} \cdot \overline{f}^T \right) \cdot \overline{x} =
\]

\[
\left( \overline{f} \cdot \overline{G(R_s)} \cdot \overline{f}^T + \sum_{\gamma_x + \gamma_y + \gamma_z = 2} \overline{Z}^w_{\gamma_x \gamma_y \gamma_z} \right) \cdot \overline{x} =
\]

\[
\left( \overline{f} \cdot \overline{G(R_s)} \cdot \overline{f}^T + \left( \overline{Z}^w_{200} + \overline{Z}^w_{110} + \overline{Z}^w_{101} + \overline{Z}^w_{020} + \overline{Z}^w_{011} + \overline{Z}^w_{002} \right) \right) \cdot \overline{x} =
\]

and, for example, the $\gamma_x = 2, \gamma_y = 0, \gamma_z = 0 \, (\overline{Z}^w_{200})$ term would be

\[
\overline{Z}^w_{200} = \overline{f}_{200} \, \overline{G}_{200} \, \overline{f}_{000}^T - 2 \overline{f}_{100} \, \overline{G}_{200} \, \overline{f}_{100}^T + \overline{f}_{000} \, \overline{G}_{200} \, \overline{f}_{200}^T
\]
Toeplitz Structure

For 1-D point interactions:

Interaction matrix is Toeplitz

\[
\begin{bmatrix}
G_0 & G_1 & G_2 & G_3 \\
G_{-1} & G_0 & G_1 & G_2 \\
G_{-2} & G_{-1} & G_0 & G_1 \\
G_{-3} & G_{-2} & G_{-1} & G_0
\end{bmatrix}
\]
Convolution Picture

Then

\[ A_u = \Pi_{bt}(A) = [1:27] \]

\[ x_z = \zeta_p(x) = \text{(see below)} \]
FFT Enhanced Multiply Speedup

From the last example,

\[ \overline{Z}^{w}_{200} = \overline{f}_{200} \overline{G}_{200} \overline{f}^{T}_{000} - 2 \overline{f}_{100} \overline{G}_{200} \overline{f}^{T}_{100} + \overline{f}_{000} \overline{G}_{200} \overline{f}^{T}_{200} \]

\( \overline{G}_{200} \overline{f}^{T}_{000} \), \( \overline{G}_{200} \overline{f}^{T}_{100} \), and \( \overline{G}_{200} \overline{f}^{T}_{200} \) can now be realized in

- \( \mathcal{O}(N \log N) \) complexity
- \( \mathcal{O}(N) \) memory storage, and
- 1-D FFT

**Full CG solution:** \( \mathcal{O}(KN_T N \log N) \) complexity, where

- \( K \) is the number of iteration
- \( N_T \) is the number of terms in the Taylor series expansion
- \( N \) is the number of particles

<table>
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<tr>
<th>Order ( \gamma )</th>
<th>Terms ( \overline{G}_{\gamma_1 \gamma_2 \gamma_3} )</th>
<th>( N_T )</th>
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<td>5</td>
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</tbody>
</table>

Number of expansion terms and total number of FFTs for expansion order \( \gamma \).
Computation times and Kullback-Leibler distances for SMCG method for $\gamma=0-5$ with $r_d=1.1\Delta r_g$ and $N_{cube}=10000$. 
Computation times and Kullback-Leibler distances for SMCG method for $r_d=0.1–2.1\Delta r_g$ with $\gamma=2$ and $N_g=8$. 
Computation times and Kullback-Leibler distances for SMCG method for $N_g=6–14$ with $\gamma=2$ and $r_d=1.1 \Delta r_g$. 

Results
Results

Radar Cross Section ($\sigma$) for increasing accurate approximations.
Comments & Conclusion

– The effective permittivity of randomly oriented collections of discrete spheroidal inclusions was obtained.

– The SMCG Method was extended to 3-D
  • Iterative solution in $O(KN_TN \log_2 N)$
  • Memory allocation is also improved to $O(N_TN)$
  • Speedup of > 20-30 times while results are within < 1% accurate

– A new $O(N \log N)$ FFT-based method to expedite matrix-vector multiplies involving multilevel block-Toeplitz (MBT) matrices was presented.

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