

Rigorous Analysis of Double-Negative Materials with the Multilevel Fast Multipole Algorithm

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Abstract — We present rigorous analysis of double-negative materials (DNMs) with surface integral equations and the multilevel fast multipole algorithm (MLFMA). Accuracy and efficiency of numerical solutions are investigated when DNMs are formulated with two recently developed formulations, i.e., the combined tangential formulation (CTF) and the electric and magnetic current combined-field integral equation (JMCFIE). Simulation results on canonical objects are consistent with previous results in the literature on ordinary objects. MLFMA is also parallelized to solve extremely large electromagnetics problems involving DNMs.

Index Terms — Double-negative materials, metamaterials, multilevel fast multipole algorithm, surface integral equations.

I. INTRODUCTION

Double-negative materials (DNMs) are commonly used as simplified models of metamaterials at resonance frequencies [1]. Specifically, a metamaterial structure at a resonance frequency can be modeled (homogenized [2]) as a homogeneous object with negative permittivity and permeability. Using the equivalence principle, a DNM can be formulated with surface integral equations, which can be discretized and solved numerically. Recently, various surface formulations,

such as the Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) formulation [3], the Müller formulation [4], and the electric and magnetic current combined-field integral equation (JMCFIE) [5], have been used to analyze DNMs [6],[7]. It has been shown that homogenization can provide fast analysis of metamaterial structures before their detailed analysis via full-wave solvers [8].

Although electromagnetics problems obtained via homogenization are relatively easy compared to the original problems, their efficient solutions may not be trivial. Surface integral equations require only the discretization of boundaries, but the resulting matrix equations can be very large because realistic metamaterials are usually large with respect to wavelength. Hence, fast and efficient methods, such as the multilevel fast multipole algorithm (MLFMA) [9]–[13], are required for the solution of large metamaterial problems, even when they are homogenized. Applying MLFMA to homogeneous materials, including DNMs, is straightforward, but the number of iterations must be small for efficient solutions, and thus the choice of the surface formulation is critical for efficient solutions.

In this paper, we present iterative solutions of DNMs using MLFMA. Problems are formulated with two recently developed formulations, namely, the combined tangential formulation (CTF) [14] and JMCFIE [5], and discretized with the Rao-Wilton-Glisson (RWG) functions [15]. Accuracy and efficiency of numerical solutions are investi-

gated on canonical problems involving the sphere geometry. We show that the conventional JMC-FIE (with $\alpha = 0.5$ combination parameter) provides efficient solutions but relatively inaccurate results. In addition, accuracy of simulations can significantly be improved using CTF, instead of JMCFIE. These observations are consistent with earlier results obtained for ordinary materials [16]. We also show that the combination parameter of JMCFIE can be increased towards unity to improve the accuracy of JMCFIE, without sacrificing the efficiency. Finally, MLFMA is parallelized using the hierarchical partitioning strategy [17] to solve very large problems involving DNMs. The resulting implementation based on JMCFIE (with high combination parameter) and parallel MLFMA seems to be a suitable solver for the fast and accurate analysis of DNMs.

II. NUMERICAL SOLUTIONS OF SURFACE FORMULATIONS

For homogeneous penetrable objects, discretizations of surface formulations lead to $2N \times 2N$ dense matrix equations in the form of

$$\begin{bmatrix} \bar{\mathcal{Z}}^{(11)} & \bar{\mathcal{Z}}^{(12)} \\ \bar{\mathcal{Z}}^{(21)} & \bar{\mathcal{Z}}^{(22)} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{v}^{(1)} \\ \mathbf{v}^{(2)} \end{bmatrix}. \quad (1)$$

Using JMCFIE and a Galerkin discretization,

$$\bar{\mathcal{Z}}^{(ab)}[m, n] = \int_{S_m} d\mathbf{r} \mathbf{t}_m(\mathbf{r}) \cdot \mathcal{Z}^{(ab)}\{\mathbf{b}_n\}(\mathbf{r}) \quad (2)$$

for $a = 1, 2$ and $b = 1, 2$, where \mathbf{t}_m and \mathbf{b}_n represent the testing and basis functions with spatial supports of S_m and S_n , respectively, for $m, n = 1, 2, \dots, N$. The combined operators are defined as

$$\begin{aligned} \mathcal{Z}^{(11)} = \mathcal{Z}^{(22)} = & -\alpha \hat{\mathbf{n}} \times \hat{\mathbf{n}} \times (\mathcal{T}_o + \mathcal{T}_i) \\ & + (1 - \alpha) \hat{\mathbf{n}} \times (\mathcal{K}_o - \mathcal{K}_i) - (1 - \alpha) \mathcal{I} \end{aligned} \quad (3)$$

$$\begin{aligned} \mathcal{Z}^{(12)} = & (1 - \alpha) \hat{\mathbf{n}} \times (\eta_o^{-1} \mathcal{T}_o - \eta_i^{-1} \mathcal{T}_i) \\ & + \alpha \hat{\mathbf{n}} \times \hat{\mathbf{n}} \times (\eta_o^{-1} \mathcal{K}_o + \eta_i^{-1} \mathcal{K}_i) \\ & - \frac{1}{2} \alpha (\eta_o^{-1} - \eta_i^{-1}) \hat{\mathbf{n}} \times \mathcal{I} \end{aligned} \quad (4)$$

$$\begin{aligned} \mathcal{Z}^{(21)} = & -(1 - \alpha) \hat{\mathbf{n}} \times (\eta_o \mathcal{T}_o - \eta_i \mathcal{T}_i) \\ & - \alpha \hat{\mathbf{n}} \times \hat{\mathbf{n}} \times (\eta_o \mathcal{K}_o + \eta_i \mathcal{K}_i) \\ & + \frac{1}{2} \alpha (\eta_o - \eta_i) \hat{\mathbf{n}} \times \mathcal{I}, \end{aligned} \quad (5)$$

where $\alpha \in [0, 1]$ is the combination parameter, $\hat{\mathbf{n}}$ is the unit normal vector at the observation point \mathbf{r} , and $\eta_u = \sqrt{\mu_u}/\sqrt{\epsilon_u}$ is the wave impedance in the outer ($u = o$) and inner ($u = i$) media. The integro-differential operators are defined as

$$\begin{aligned} \mathcal{T}_u\{\mathbf{b}_n\}(\mathbf{r}) = & \frac{i}{k_u} \int_{S_n} d\mathbf{r}' \nabla' \cdot \mathbf{b}_n(\mathbf{r}') \nabla g_u(\mathbf{r}, \mathbf{r}') \\ & + ik_u \int_{S_n} d\mathbf{r}' \mathbf{b}_n(\mathbf{r}') g_u(\mathbf{r}, \mathbf{r}') \end{aligned} \quad (6)$$

$$\mathcal{K}_u\{\mathbf{b}_n\}(\mathbf{r}) = \int_{PV, S_n} d\mathbf{r}' \mathbf{b}_n(\mathbf{r}') \times \nabla' g_u(\mathbf{r}, \mathbf{r}'), \quad (7)$$

where PV indicates the principal value of the integral, $k_u = \omega \sqrt{\epsilon_u} \sqrt{\mu_u}$ is the wavenumber, and

$$g_u(\mathbf{r}, \mathbf{r}') = \frac{\exp(ik_u |\mathbf{r} - \mathbf{r}'|)}{4\pi |\mathbf{r} - \mathbf{r}'|} \quad (8)$$

denotes the homogeneous-space Green's function in the phasor domain using the $e^{-i\omega t}$ time dependence. The elements of the right-hand-side vectors in (1) are derived similarly as

$$v_m^{(a)} = \int_{S_m} d\mathbf{r} \mathbf{t}_m(\mathbf{r}) \cdot \boldsymbol{\psi}^{(a)}(\mathbf{r}) \quad (9)$$

for $a = 1, 2$, where

$$\begin{aligned} \boldsymbol{\psi}^{(1)}(\mathbf{r}) = & -(1 - \alpha) \hat{\mathbf{n}} \times \mathbf{H}^{inc}(\mathbf{r}) \\ & + \alpha \eta_o^{-1} \hat{\mathbf{n}} \times \hat{\mathbf{n}} \times \mathbf{E}^{inc}(\mathbf{r}) \end{aligned} \quad (10)$$

$$\begin{aligned} \boldsymbol{\psi}^{(2)}(\mathbf{r}) = & (1 - \alpha) \hat{\mathbf{n}} \times \mathbf{E}^{inc}(\mathbf{r}) \\ & + \alpha \eta_o \hat{\mathbf{n}} \times \hat{\mathbf{n}} \times \mathbf{H}^{inc}(\mathbf{r}). \end{aligned} \quad (11)$$

In (10) and (11), \mathbf{E}^{inc} and \mathbf{H}^{inc} represent the incident electric and magnetic fields created by external sources located in the outer medium.

JMCFIE is a mixed formulation involving directly and rotationally tested electromagnetic fields. Using a Galerkin discretization (using the same set of the RWG functions as the basis and testing functions), JMCFIE involves a well-tested identity operator, i.e.,

$$\begin{aligned} \bar{\mathbf{I}}_{mn} = & \int_{S_m} d\mathbf{r} \mathbf{t}_m(\mathbf{r}) \cdot \mathbf{b}_n(\mathbf{r}) \\ = & \int_{S_m} d\mathbf{r} \mathbf{t}_m(\mathbf{r}) \cdot \int_{S_n} \delta(\mathbf{r}, \mathbf{r}') \mathbf{b}_n(\mathbf{r}'), \end{aligned} \quad (12)$$

which is a major error source for low-order discretizations [18]. CTF can be seen as a special case of JMCFIE and it is obtained by setting

$\alpha = 1$ in (3)–(5), (10), and (11). Note that well-tested identity operators disappear in CTF; this explains why it is more accurate than JMCFIE.

Employing the conventional formulations, such as PMCHWT and JMCFIE, for DNMs is extensively discussed in [6],[7]. Using $k_u = \omega\sqrt{\epsilon_u}\sqrt{\mu_u}$ and $\eta_u = \sqrt{\mu_u}/\sqrt{\epsilon_u}$ leads to negative wavenumber and positive wave impedance when the permittivity (ϵ_u) and permeability (μ_u) are negative. In order to construct a tree structure for a DNM, we use the absolute value of k_u in the excess bandwidth formula, i.e.,

$$\tau_{l,u} \approx 1.73|k_u|a_l + 2.16(d_0)^{2/3}(|k_u|a_l)^{1/3}, \quad (13)$$

to determine truncation numbers $\tau_{l,u}$ and samples on the unit sphere. In (13), a_l is the box size at level l and d_0 is the number of accurate digits for the far-field interactions.

III. NUMERICAL RESULTS

In order to test the accuracy and efficiency of solutions of DNMs with MLFMA, we consider increasingly large scattering problems involving a sphere of radius 0.3 m. The object is located in free space and illuminated by plane waves at various frequencies. Problems are formulated with CTF and JMCFIE and discretized with the RWG functions on $\lambda_o/10$ triangles, where λ_o is the wavelength in the host medium (free space). Both near-field and far-field interactions are calculated with maximum 1% error. Solutions are performed using the biconjugate-gradient-stabilized (BiCGStab) algorithm [19] accelerated with MLFMA. Iterative convergences are also accelerated with the four-partition block-diagonal preconditioner (4PBDP) [16] for the conventional JMCFIE ($\alpha = 0.5$).

Fig. 1 presents the solution of a small scattering problem involving a sphere of radius 0.3 m at 500 MHz. Both the relative permittivity and permeability of the sphere are selected as -2.0 . The sphere is illuminated by a plane wave from the top and the problem is formulated with CTF. For numerical solutions, the problem is discretized with 1860 unknowns. Fig. 1 depicts the total electric field in the vicinity of the sphere on the E-plane for the inner and outer problems. The maximum electric field value is normalized to 0 dB. For the inner/outer problem, the equivalent currents

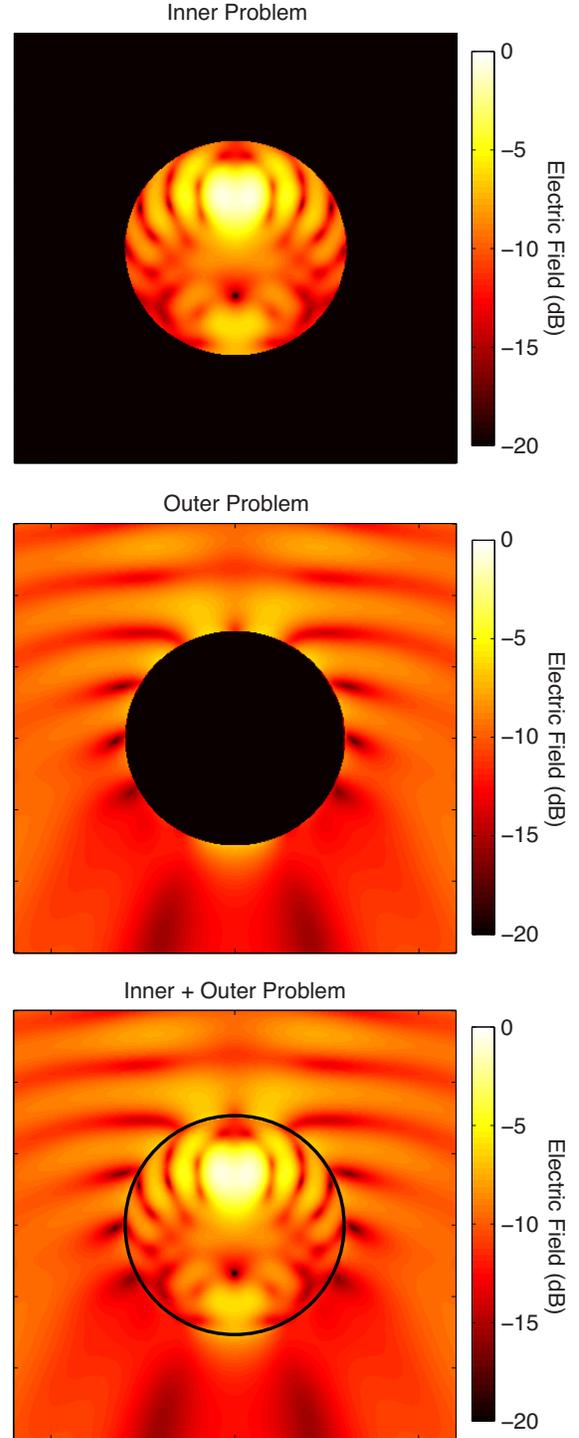


Fig. 1. Solution of a scattering problem involving a sphere of radius 0.3 m at 500 MHz. Both the relative permittivity and permeability of the sphere are -2.0 .

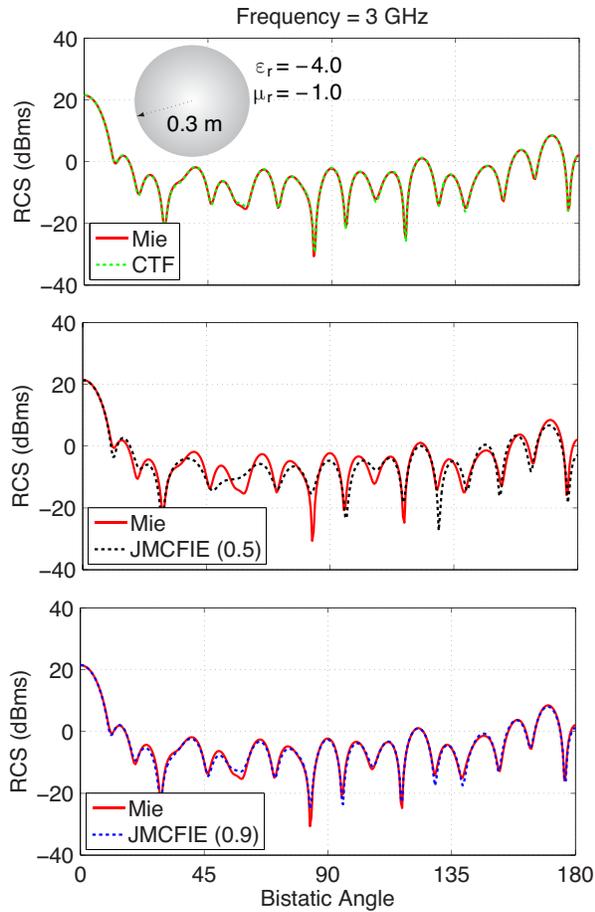


Fig. 2. Solutions of a scattering problem involving a sphere of radius 0.3 m at 3 GHz. The relative permittivity and permeability of the sphere are -4.0 and -1.0 , respectively.

provided by MLFMA are allowed to radiate into a homogeneous space with the electrical parameters of the inner/outer medium assumed everywhere. Hence, for the inner/outer problem, any radiation outside/inside the sphere can be interpreted as numerical error. It can be observed that these unwanted radiations are below -20 dB, verifying the high accuracy of the solution. As also depicted in Fig. 1, the complete plot can be obtained by superimposing the plots for the inner and outer problems. It is remarkable that field values become maximum in the upper part of the sphere as a result of the negative refractive index of the object.

Fig. 2 presents the solution of a scattering problem involving a sphere of radius 0.3 m at

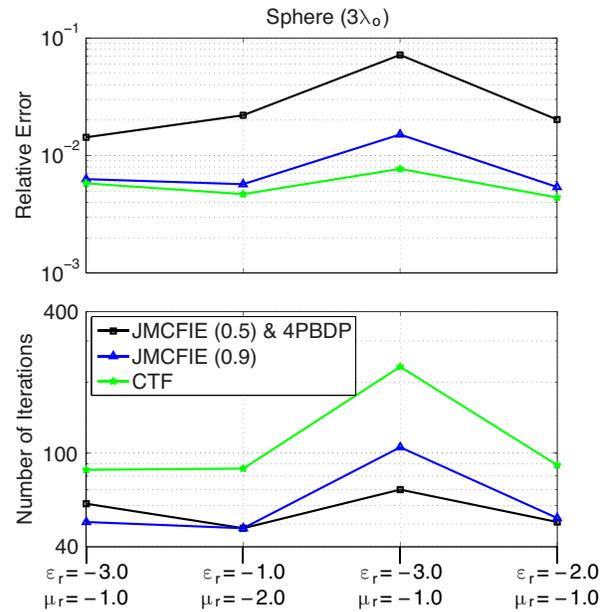


Fig. 3. The relative error and the number of BiCGStab iterations (for 10^{-3} residual error) required in numerical solutions of scattering problems involving a sphere of radius 0.3 m at 3 GHz.

3 GHz. In this problem, the relative permittivity and permeability of the sphere are selected as -4.0 and -1.0 , respectively. For numerical solutions, the problem is discretized with 65,724 unknowns. Fig. 2 depicts the radar cross section (RCS) on the E-plane as a function of the bistatic observation angle from 0° to 180° , where 0° and 180° correspond to the forward-scattering and backscattering directions, respectively. Computational values obtained with CTF, the conventional JMCFIE ($\alpha = 0.5$), and JMCFIE with a high combination parameter ($\alpha = 0.9$) are compared to the analytical Mie-series results. It can be observed that CTF results agree very well with the analytical results. However, the same level of accuracy is not obtained with the conventional JMCFIE. In addition, as also depicted in Fig. 2, increasing the combination parameter to 0.9 significantly improves the accuracy.

For a more quantitative comparison of the formulations, Fig. 3 presents the results of scattering problems involving a sphere with different material properties. A sphere of radius 0.3 m is again investigated at 3 GHz and discretized with 65,724

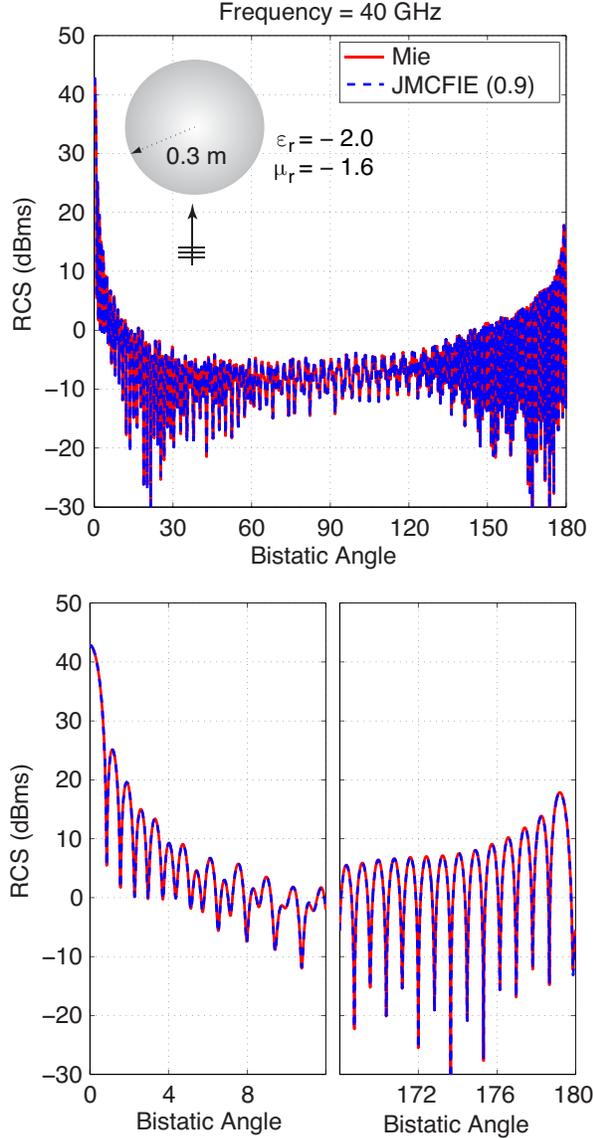


Fig. 4. Solution of a scattering problem involving a sphere of 0.3 m at 40 GHz. The relative permittivity and permeability of the sphere are -2.0 and -1.6 , respectively.

unknowns. The first plot of Fig. 3 depicts the relative error in the far-zone electric field obtained with different formulations. To find the relative error, the co-polar electric field in the far-zone on the E-plane is sampled at $\pi/360$ intervals, i.e., we compute

$$f[n] = \lim_{r \rightarrow \infty} \{r E_{\varphi}(r, \varphi[n])\}, \quad (14)$$

where $\varphi[n] = (n-1)\pi/360$ for $n = 1, 2, \dots, 361$. Then, the error is defined as

$$\Delta = \frac{\|\mathbf{f}_C - \mathbf{f}_A\|}{\|\mathbf{f}_A\|}, \quad (15)$$

where $\|\cdot\|$ represents the 2-norm and \mathbf{f}_C and \mathbf{f}_A are vectors of 361 elements containing the computational and analytical values, respectively. It can be observed that the relative error for the conventional JMCFIE ($\alpha = 0.5$) is generally higher than 1%, which may not be acceptable. As also shown in the same plot, the accuracy is significantly improved by using CTF or increasing the amount of CTF in JMCFIE, i.e., using JMCFIE with $\alpha = 0.9$, instead of the conventional JMCFIE. As complementary data, the second plot of Fig. 3 depicts the number of BiCGStab iterations for 0.001 residual error. Iterative solutions of the conventional JMCFIE ($\alpha = 0.5$) are accelerated with 4PBDP; but this preconditioner is not useful for CTF and JMCFIE with $\alpha = 0.9$. It can be observed that JMCFIE (both with $\alpha = 0.5$ and with $\alpha = 0.9$) provides very efficient solutions, compared to CTF. Considering the results in both plots of Fig. 3, JMCFIE with $\alpha = 0.9$ seems to be a good choice for efficient and accurate solutions.

Finally, Fig. 4 presents the solution of a large scattering problem involving a sphere of radius 0.3 m at 40 GHz. The relative permittivity and permeability of the sphere are -2.0 and -1.6 , respectively. The problem is formulated with JMCFIE using $\alpha = 0.9$ and discretized with 11,702,832 unknowns. MLFMA is parallelized into 64 processes on a cluster of Intel Xeon Nehalem quad-core processors with 2.80 GHz clock rate. The total time including the setup and 176 iterations (for 0.005 residual error) is approximately 10 hours. Fig. 4 depicts the bistatic RCS values on the z - x plane as a function of the bistatic angle θ from 0° to 180° . RCS values around the forward-scattering (0°) and backscattering (180°) directions are also focused in separate plots. It can be observed that the computational values obtained by using JMCFIE and parallel MLFMA agree very well with the analytical results. For this large-scale problem, the relative error in (15) is found to be 0.21%.

IV. CONCLUSIONS

This paper presents the analysis of DNMs with surface integral equations and MLFMA. Numerical results obtained with conventional formulations are in agreement with previous results obtained for ordinary materials. Numerical experiments on canonical objects show that JMCFIE with $\alpha = 0.9$ is a good choice for efficient and accurate solutions.

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