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First results of using weighted discretization in the ADDA code

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In order to describe scattering and absorption of electromagnetic waves by an arbitrary shaped particle [1], the discrete dipole approximation (DDA) is widely used. It consists in a discretization of the particle volume using a set of small voxels (dipoles), Figure 1a. Assuming the electric fields to be constant inside each voxel, the corresponding value \mathbf{E}_i for a given voxel is determined from a linear system of equations, which takes into account the incident field $\mathbf{E}_i^{\text{inc}}$ and interactions $\overline{\mathbf{G}}_{ij}$ with other voxels of the set as

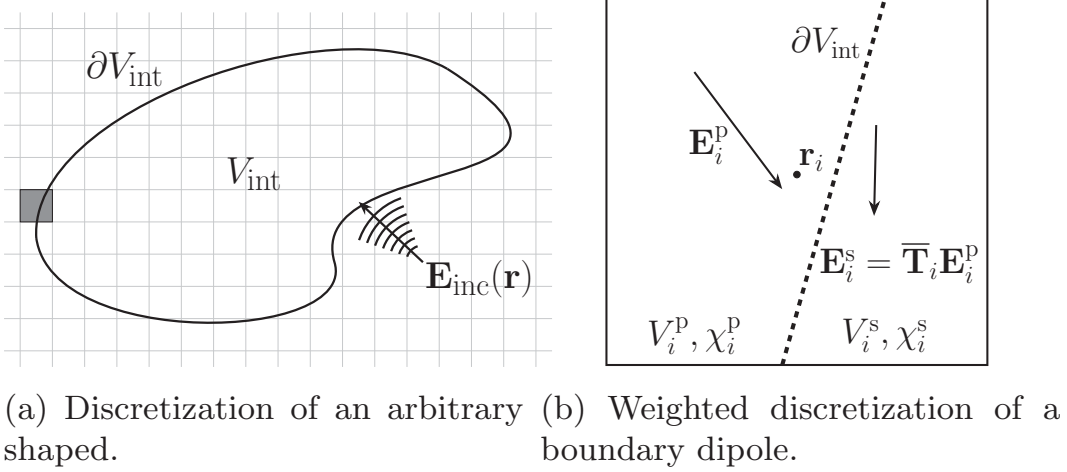
$$\mathbf{E}_i = \mathbf{E}_i^{\text{inc}} + \sum_{j \neq i} \overline{\mathbf{G}}_{ij} V_j \chi_j \mathbf{E}_j + (\overline{\mathbf{M}}_i - \overline{\mathbf{L}}_i) \chi_i \mathbf{E}_i, \quad (1)$$

where χ_i is the susceptibility associated with the relative (to the host medium) refractive index m of the scatterer while $\overline{\mathbf{L}}_i$ and $\overline{\mathbf{M}}_i$ are, respectively, the self-term dyadic and a correction associated to the finiteness of the voxel volume V_i . The traditional discretization scheme (TD) uses identical cubical sub-volumes as voxels. However, due to the mismatch of some voxels with the boundary of the scatterer (i.e., staircasing effect), shape errors are expected for most of the particles [2].

Thus, a weighted discretization (WD) is proposed to reduce these errors without changing the regular rectangular grid. First, the simplest option is to consider the effective medium approximation [3] to modify the susceptibility of these boundary voxels. Second, Piller [4] proposed an alternative based on the splitting of these voxels into two different parts (Figure 1b) by a plane interface: a primary part (p), which contains the voxel center \mathbf{r}_i , and a secondary one (s). The electric fields in both

domains are linearly related $\mathbf{E}_i^s = \bar{\mathbf{T}}_i \mathbf{E}_i^p$ through the boundary-condition tensor $\bar{\mathbf{T}}_i$. Therefore, an effective susceptibility $\bar{\chi}_i^e$ (2) is determined from a weighted average of the susceptibility, based on the volume fraction $f_i \triangleq V_i^p/V_i$ of the voxel:

$$\bar{\chi}_i^e \triangleq f_i \chi_i^p \bar{\mathbf{I}} + (1 - f_i) \chi_i^s \bar{\mathbf{T}}_i. \quad (2)$$



(a) Discretization of an arbitrary (b) Weighted discretization of a boundary dipole.

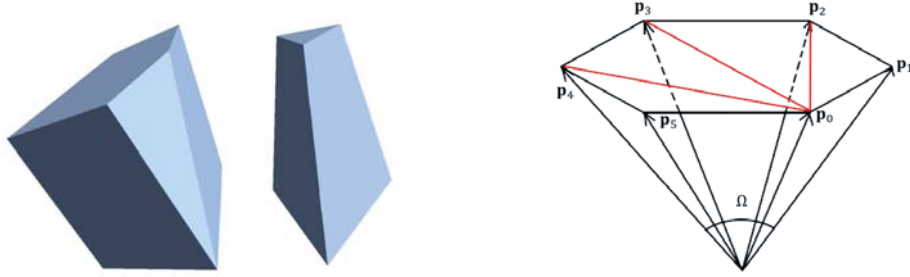
Figure 1: Weighted discretization applied to the particle.

Although the self-term dyadic $\bar{\mathbf{L}}_i$ is determined as the sum of both parts as $\bar{\mathbf{L}}_i = \bar{\mathbf{L}}_i^p + \bar{\mathbf{L}}_i^s$, some cumbersome computational geometry is used [5] to evaluate it for each part. In the DDA framework, the general expression for the self-term dyadic is given by the following integral form [1]

$$\bar{\mathbf{L}}(\partial V_i, \mathbf{r}_i) \triangleq \oint_{\partial V_i} \frac{\hat{\mathbf{n}}(\mathbf{r}') \otimes (\mathbf{r}' - \mathbf{r}_i)}{|\mathbf{r}_i - \mathbf{r}'|^3} d^2 \mathbf{r}' \quad (3)$$

Since the boundary ∂V_i of any polyhedron consists of several facets, one only needs to compute the contribution $\bar{\mathbf{L}}(\mathcal{S}_\ell^i, \mathbf{r}_i)$ of the self-term dyadic over a single facet \mathcal{S}_ℓ^i with vertices $\{\mathbf{p}_k\}$ and solid angle Ω (as viewed from \mathbf{r}_i). This contribution is deduced after some algebra, using $\hat{\mathbf{q}}_k \triangleq (\mathbf{p}_{k+1} - \mathbf{p}_k)/|\mathbf{p}_{k+1} - \mathbf{p}_k|$, to be [5]

$$\bar{\mathbf{L}}(\mathcal{S}_\ell^i, \mathbf{r}_i) = \Omega \hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_i + \sum_{k=0}^{n-1} \ln \left(\frac{\mathbf{p}_{k+1} \cdot \hat{\mathbf{q}}_k + |\mathbf{p}_{k+1}|}{\mathbf{p}_k \cdot \hat{\mathbf{q}}_k + |\mathbf{p}_k|} \right) \hat{\mathbf{q}}_k \times \hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_i. \quad (4)$$



(a) Boundary voxel cut by a plane (b) Facet of the boundary voxel interface. with vertices \mathbf{p} and solid angle Ω .

Figure 2: Computational geometry considerations for $\bar{\mathbf{L}}_i$, reproduced from [5].

Along with the above modifications, the term $(\bar{\mathbf{M}}_i - \bar{\mathbf{L}}_i) \chi_i \mathbf{E}_i$ in (1) becomes $\left[(\bar{\mathbf{M}}_i^{\text{p}} - \bar{\mathbf{L}}_i^{\text{p}}) \chi_i^{\text{p}} + (\bar{\mathbf{M}}_i^{\text{s}} - \bar{\mathbf{L}}_i^{\text{s}}) \chi_i^{\text{s}} \bar{\mathbf{T}}_i \right] \mathbf{E}_i$. $\bar{\mathbf{M}}_i^{\text{p,s}}$ are hard to evaluate, but they decrease with voxel size d unless the particle boundary comes very close to its center. Thus, they can be either neglected or replaced by the traditional expression $\bar{\mathbf{M}}_i$ without significant loss of accuracy (since the number of boundary voxels is relatively small).

In order to show how the weighted discretization improves the simulation accuracy, errors with respect to the Mie theory for both traditional and weighted discretization schemes are investigated for spheres with radius $R = \lambda/2$ and λ (where λ is the incident wavelength). For that, the light scattering code ADDA [6] is used, for which a prototype of the weighted discretization has been implemented on a separate branch [5]. This prototype is compared to the main version of ADDA employing traditional discretization. Considering simple spheres of refractive index $m = 1.33$ and $m = 2 + i$ in vacuum, the relative errors on extinction and scattering efficiencies were determined (using the Lorenz–Mie theory as a reference [7]) as a function of grid size along the sphere diameter (Figures 3 & 4).

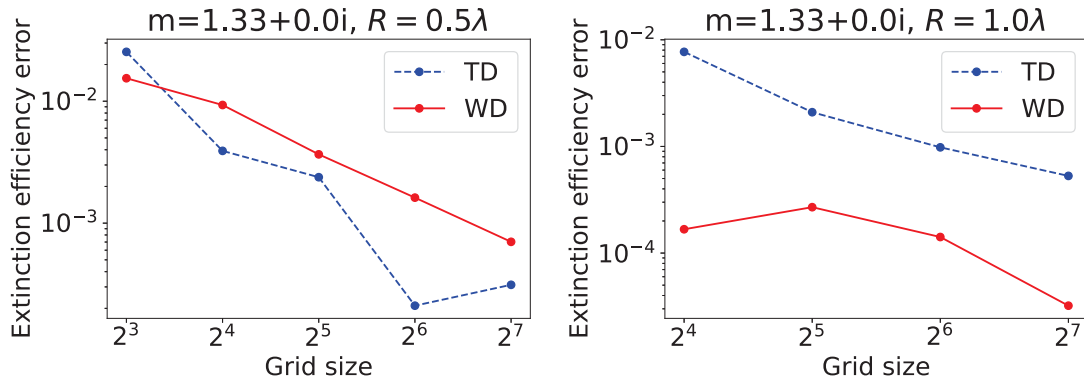


Figure 3: Error of extinction efficiencies for non-absorbing spheres versus number of voxels per diameter in log-log scale.

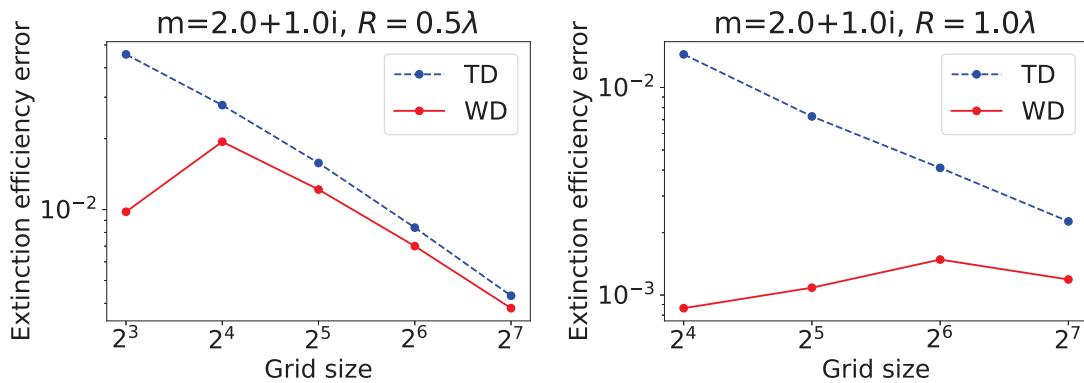


Figure 4: Error of extinction efficiencies for absorbing spheres versus number of voxels per diameter in log-log scale.

In some cases, WD greatly improves the accuracy of the DDA, but this improvement is not universal. That is partially expected. First, the WD addresses only the shape errors, this will not make a significant difference, when discretization errors dominate. Second, TD is more sophisticated than it seems, because ADDA applies so-called volume correction, which stretches the whole scale of the voxel set to exactly match the volume of the original particle. This is known to be especially efficient for small particles, where the total size (or volume) of the particle comes at some power as a factor into any scattering quantity.

We will provide data at the conference for a wider range of particles (m , R , and shape) and DDA variants. The latter will include the TD without volume correction and combination of various discretization regimes with the integration of Green's tensor (IGT). It has been hypothesized that coupling IGT and WD should lead to a quadratic convergence (error vs. voxel size) [2].

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