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Improved volume integral equation method for computing optical properties of black carbon-containing aerosol particles

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Black carbon (BC) is a light-absorbing carbonaceous aerosol emitted from combustions of fossil fuels and biomasses and is estimated as the second most important contributor to positive climate forcing after the carbon dioxide. BC-containing aerosol particles in the atmosphere are microscopically observed to be the fractal-like aggregates of primary BC-spherules. The fractal aggregate of BC-spherules may be mixed with non-absorbing (or weakly absorbing) compounds that forms morphologically complex "BC-containing particle". In the field of atmospheric chemistry and physics, an accurate light-scattering code for BC-containing particles is required in two important applications: 1) reliable algorithm for in-situ optical measurements and remote sensing of their physical properties (e.g., size distribution, mixing state, shape; 2) developing an accurate parameterization scheme for predicting mass absorption efficiency of BC from the physical properties of BC-containing particles given by a chemical transport model. In this work, we propose a robust scheme of volume integral equation method (VIEM) for computing light scattering and absorption by arbitrary BC-containing particles. In conventional scheme, the entire volume of each particle is uniformly approximated as a collection of small volume elements (dipoles) on a cubic lattice (CL). In the proposed scheme, each BC-spherule is represented by a spherical dipole with original size, while remaining particle volume occupied by non-absorbing compounds is approximated by a collection of uniform dipoles on a CL. We call this as Spherule-Retained-Cubic-Lattice (SRCL) scheme. For several model BC-containing particles, positive absorption bias of $\sim$30% persistent in conventional CL scheme is successfully eliminated in the SRCL scheme, as shown by comparison with numerically exact T-matrix computations. For SRCL scheme, we introduce an efficient algorithm for matrix-vector product (MVP) in Krylov subspace iteration. The MVP is equivalent to evaluating electromagnetic interactions between all possible pairs of dipoles. In our modified MVP algorithm, the computation is decomposed into three distinct parts: 1) "BC-BC" interactions; 2) "BC-Coat" interaction; 3) "Coat-Coat" interactions; where "BC" and "Coat" represent dipoles corresponding to BC-spherule and non-absorbing volume, respectively. The total memory required for the modified MVP algorithm can be several orders of magnitude less than that for default MVP algorithm. Furthermore, we also discuss possible use of FFT in the modified MVP algorithm.