Postdoc position at CORIA

Project

Title: Accelerating iterative solvers in the discrete dipole approximation
Keywords: light scattering, discrete dipole approximation, iterative methods
Part of project: RADDAERO (Chair of Excellence of Normandy Region)
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Abstract

Many scientifical and technological applications, related to remote sensing and non-invasive characterization, rely on rigorous methods to simulate scattering of electromagnetic waves by various particles. The discrete dipole approximation (DDA) is one of the most general methods for such simulations, widely used through a few open-source implementations, e.g., ADDA code. The method employs volume discretization of the particle, thus being applicable to arbitrary inhomogeneous scatterers. The only drawback is relatively large computational costs despite many existing optimizations.

This postdoc project aims to further improve the efficiency of the DDA simulations, focusing on the optimization of the iterative solution of the underlying linear systems. This includes various initial guesses based on approximate solutions of the same light-scattering problem, block-iterative methods for simultaneous solution of multiple linear systems (e.g., different orientations of the same particle), and circulant preconditioners for large particles. Moreover, the project involves implementation of operator-based regularization, which has a potential to drastically accelerate the DDA for metallic nanoparticles and to provide rigorous simulations for the case of excitation sources placed inside a particle (e.g., for simulation of near-field radiative heat transfer). Overall, these developments will enable wider use of the DDA and, ultimately, lead to the adoption of rigorous simulations in applications, where it has not been previously feasible.

Detailed description

Interaction of electromagnetic waves (from X-ray to the visible and radar wavelengths) with various particles and particle systems is one of the cornerstones of the modern science, having multiple technological applications. The latter include remote sensing of aerosols (critical for weather and climate modelling), non-invasive characterization methods for reactive fluids or biological particles (thus, critical for medical diagnostics), and 3D shape reconstruction of atomic clusters with X-ray tomography. Robust simulation capabilities are a must for all these applications. One of the general methods for such simulations is the discrete dipole approximation (DDA) [1,2]. Due to the used volume discretization, the DDA applies to (inhomogeneous) particles of arbitrary shape and internal structure with sizes from much smaller than to several tenth of wavelengths. Importantly, the existing popularity of the DDA is largely based on the availability of the open-source software packages, mainly DDSCAT and ADDA.

In particular, ADDA is a C software package with about 10 contributors [3], led by Maxim Yurkin, https://github.com/adda-team/adda. The main feature of ADDA is the ability to run on a multiprocessor system or multicore processors (parallelizing a single DDA simulation). Moreover, it incorporates many improvements of the accuracy and numerical efficiency of the DDA and is highly trusted by the community (used in more than 500 publications). Overall, ADDA provides robust, efficient, and user-friendly simulation capabilities for arbitrary shaped particles in many fields from biology and nanotechnology to climate studies and astrophysics.

A critical component of the DDA is an iterative solution of a huge linear system, which optimization is the main objective of the postdoc project. The first idea is to implement initial guesses based on various approximations – recently it has been successfully used in combination with the low-contrast limit of the geometric optics [4]. This can be extended to full geometric optics (for particles of any refractive index) or one can employ various empirical corrections to the RGD theory, proposed for fractal aggregates [5]. The second idea is to use the so-called block-iterative methods [6,7] to accelerate simulations with multiple incident fields (e.g., for orientational averaging). During the preliminary work, several of such methods have been implemented at a separate development branch of ADDA, but the code is far from being production-ready, and acceleration has been rather modest so far (2-3 times for block size of several tens). The reasons for the latter are to be investigated. The third idea is to test various preconditioners, which are expected to significantly accelerate simulations for large homogeneous particles. While many of the standard preconditioners cannot be applied to the DDA due to the used FFT acceleration, so-called circulant preconditioners can [8,9]. However, the success has been so far limited to very oblate or prolate particle. These preconditioners need to be investigated for particles with comparable dimensions along all axes.

Another optimization is so-called operator preconditioning or regularization, which boils down to a quadratic function of the original integral operator [10,11]. On the one hand, the discretization of the regularized operator equation is highly non-trivial, since it involves computation of double volume integrals. For the latter, single-point approximation will definitely fail in contrast to the standard DDA with regular incident field. However, recently derived analytic formulae for integration of Green’s tensor may help here. On the other hand, if successful, such regularization should drastically improve the DDA performance for metallic nanoparticles and also allow robust and efficient simulations for the cases of excitation sources placed inside a particle. The latter will lead to robust simulation of the near-field radiative heat transfer and Casimir forces with the DDA.

The goals of the postdoc project are thus:

- Acceleration of the iterative solver using initial guesses based on geometric optics or extended RGD approximation.
- Implementation of the block-iterative methods for multiple incident fields.
- Study of circulant preconditioners to accelerate iterative solver.
- Implementation of operator-based regularization with accurate discretization and its study in various applications.
- Contributions to new releases of ADDA and development of this open-source project, in general.

Candidate's experience and training

The candidate must have completed a PhD degree and have strong background in at least one of the following: light-scattering, computational electromagnetism, or iterative methods for large linear systems. Programming skills are essential; prior experience in C/C++ or with open-source projects is a definite plus. Good command of oral and written English is necessary.

Other information

The work will be carried out at CORIA laboratory in St Etienne du Rouvray, France and can start from October 2024 (or later depending on administrative procedures). The successful candidate will be enrolled as CNRS Researcher for 1 year with potential extension for another two years, depending on the candidate's performance. The gross monthly income will be 2900€ (around 2300€ net) or larger, depending on the experience.

Send your application by e-mail to maxim.yurkin@coria.fr. Your application should include your detailed CV, a cover letter, and two letters of recommendation. The closing date for sending applications is August 31, 2024, however the position will be filled as soon as a strong candidate is found.

A limited number of applications will be selected for an oral interview (by videoconference). As the CORIA laboratory is located in a Restricted Zone (ZRR), an administrative investigation will be carried out on selected applications. This will be based on your CV and proof of identity. At the end of this investigation, which can take up to 2 months, the final candidate will be notified and can begin the administrative registration process.

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