

# 首届致远学术节 学生科研成果展示

Title : A fast method for evaluating Green's function in irregular domains with application to charge interaction in a nanopore

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Method : The algorithm is based on two-level image charges, in which the inner-layer charges are located nearby the boundary to eliminate the singularity of the induced polarization potential, and the outer-layer charges with fixed positions approximate the long-range tail of the potential.

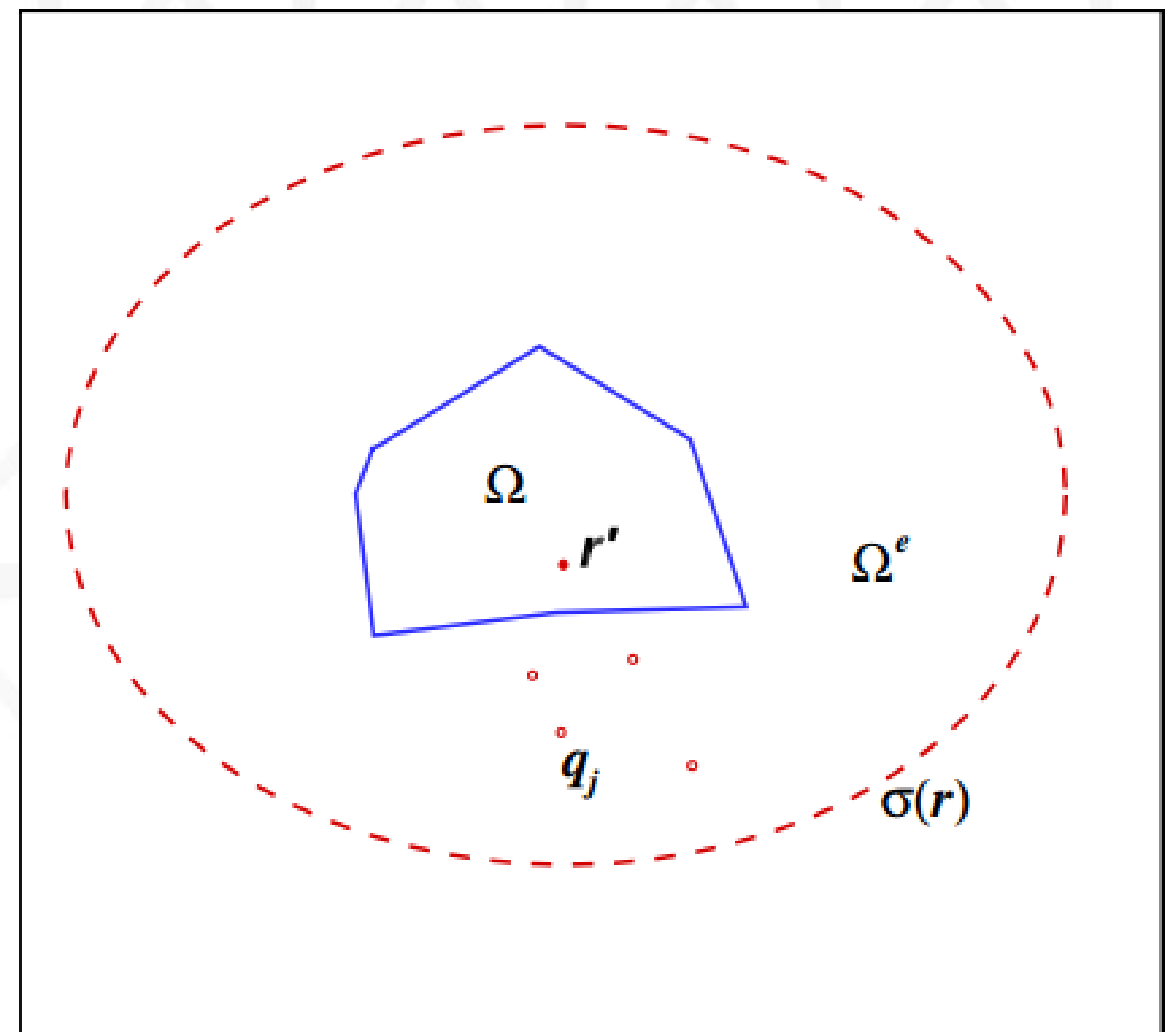


Fig. Schematic illustration for the solution of the Green's function.

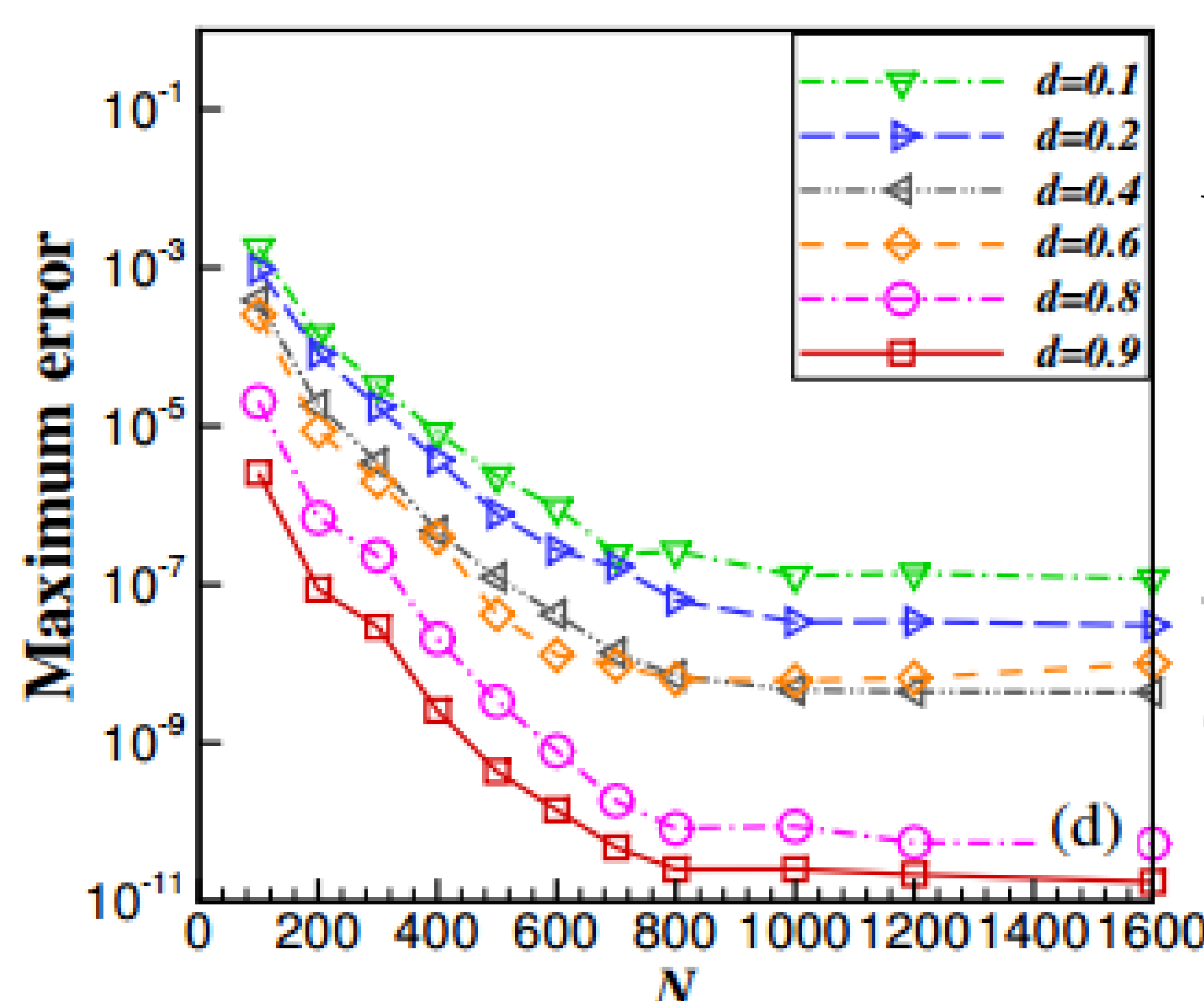
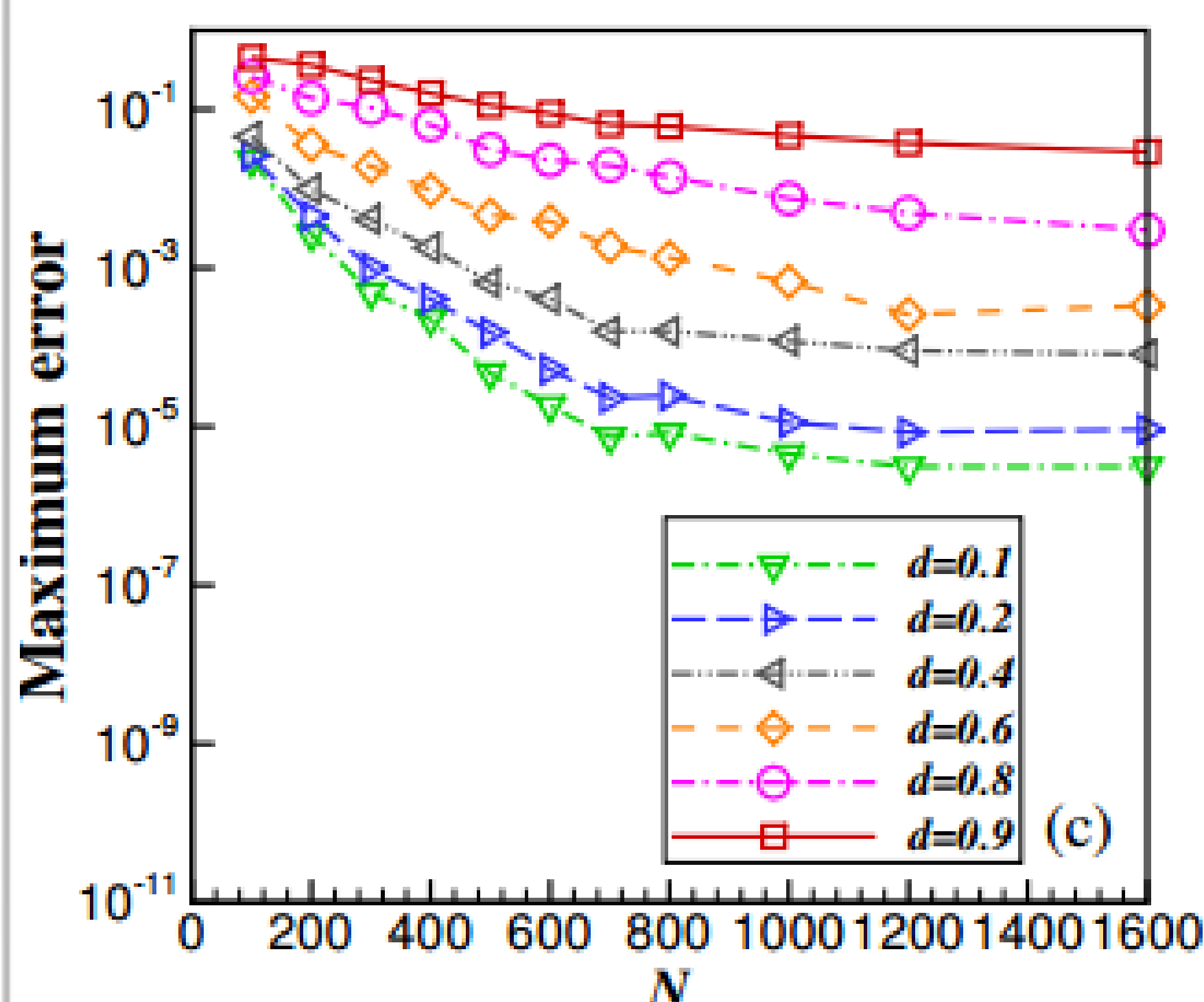
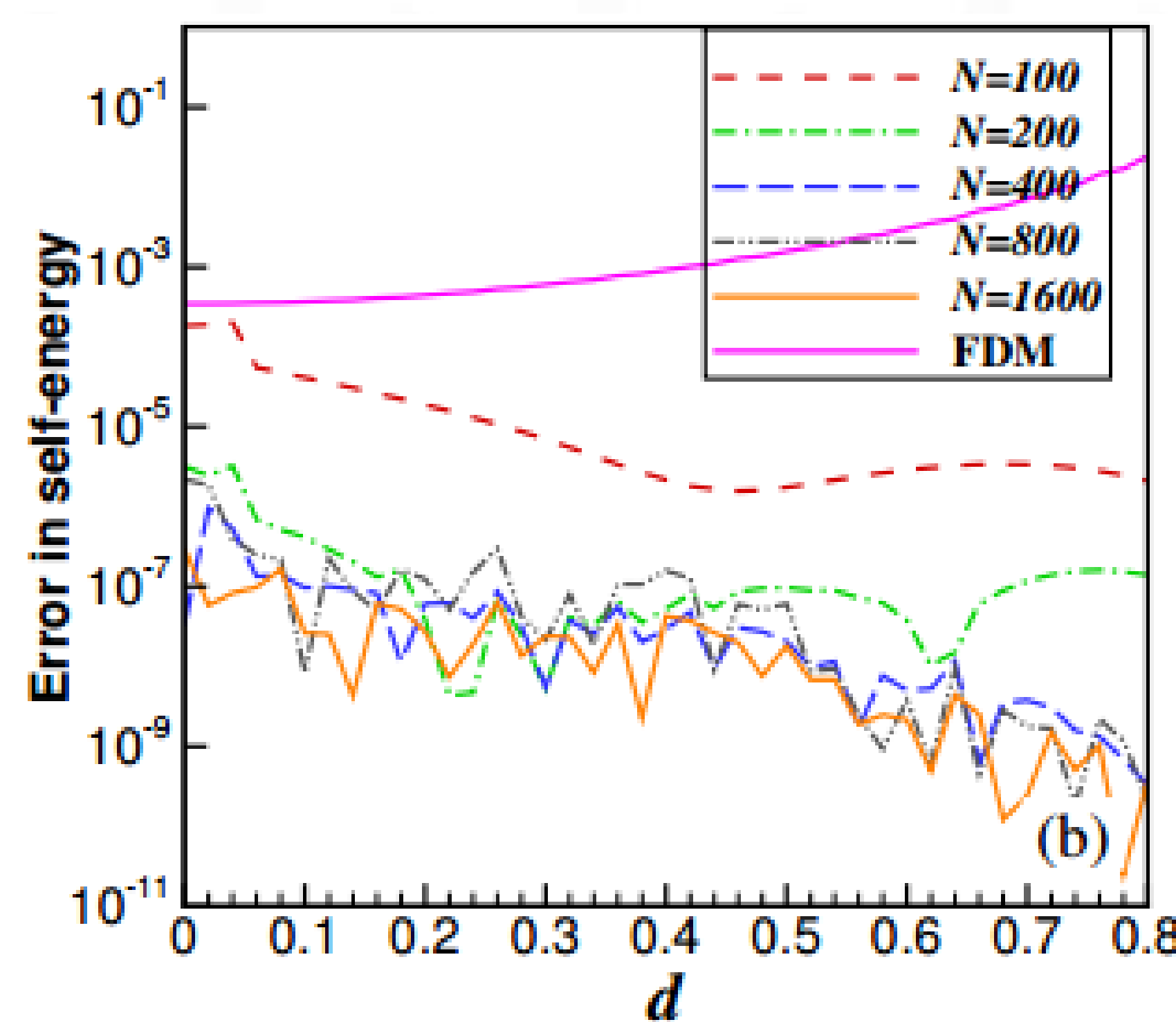
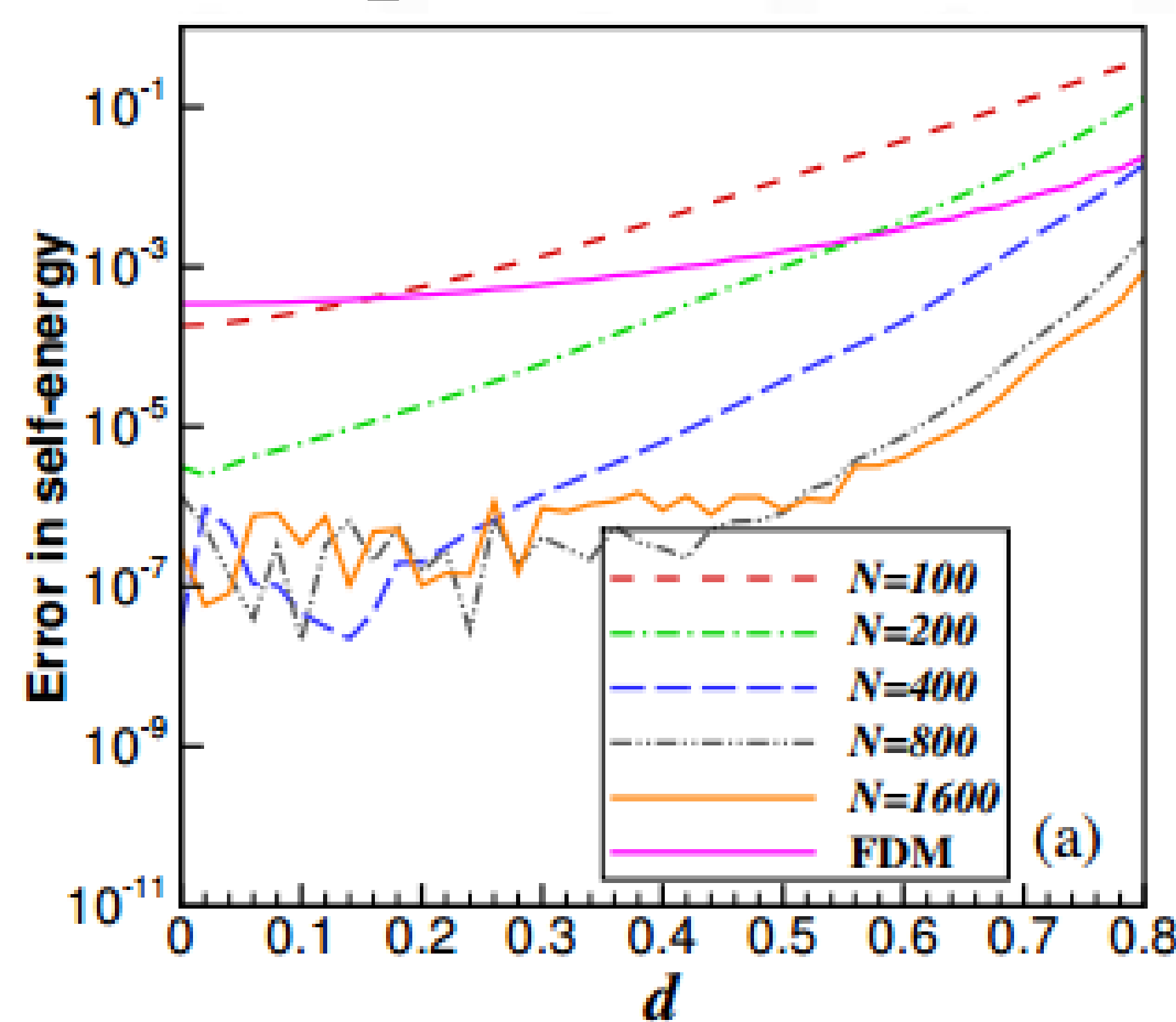


Fig. (ab) Absolute error of the self-energy for the source charge located at  $(1,1,1)d$  as function of  $d$ : (a) without and (b) with inner-layer images. (cd) Maximum error in the induced potential : (c) without and (d) with inner-layer images.

Results :

We find the number of inner-layer image charges can be very small and thus the total complexity of the algorithm is less expensive and potentially suitable for use in particle simulations.

Note:

The whole work is accepted by "communications in computational physics".

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