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Accurate and fast numerical solution of Poisson's equation for arbitrary, space-filling convex Voronoi polyhedra: near-field corrections revisited[1] AFTAB ALAM, Ames Laboratory, Ames IA, BRIAN G. WILSON, LLNL, Livermore California, DUANE D. JOHNSON, Ames Laboratory, Ames IA
— We present an accurate and rapid solution of Poisson's equation for space-filling, arbitrarily-shaped, convex Voronoi polyhedra (VP); the method is O(N), where N is the number of distinct VP representing the system. In effect, we resolve the longstanding problem of fast but accurate numerical solution of the near-field corrections (NFC), contributions to each VP potential from nearby VP – typically involving multipole-type conditionally-convergent sums, or fast Fourier transforms. Our method avoids all ill-convergent sums, is simple, accurate, efficient, and works generally, i.e., for periodic solids, molecules, or systems with disorder or imperfections. We demonstrate the method's practicality by numerical calculations compared to exactly solvable models.

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