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The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Semi-analytical solutions of boundary value problems for the stationary diffusion equation in three-dimensional canonical domains

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We present the generalized method of separation of variables (GMSV) to solve boundary value problems for the stationary diffusion equation in three-dimensional canonical domains (e.g., parallelepipeds, cylinders, spheres, spheroids, ..., and also their combinations).

The main idea of the GMSV is as follows. For the sake of definiteness, consider diffusion in a domain outside N active particles of canonical forms (sinks). One looks for the classical solution (e.g., local concentration of diffusing particles) as a superposition of N implicit expansions into basis solutions of the diffusion equation given in each curvilinear coordinate systems attached to the centers of the sinks. The unknowing coefficients of the linear combination are fixed according to Robin boundary conditions by using addition theorems to re-expand the basis solutions in one local coordinate system on the appropriate basis solutions in another local coordinate system. Although the numerical computation of the coefficients involves a matrix inversion, the use of the basis solutions specifically adapted to the symmetries of each geometric element makes the GMSV particularly efficient, especially for exterior problems. Thus, the corresponding boundary conditions are exactly satisfied by simple substitution accompanied by the use of appropriate addition theorems. As a result, the original boundary value problem with respect to a local concentration of diffusing particles reduces to resolving second kind infinite system of linear algebraic equations (ISLAE) in the Hilbert spaces of sequences. Provided the relevant matrix operator of the ISLAE is compact, the system can be truncated and numerically solved as justified by the reduction method. Moreover, we show that for some configurations of sinks the resolving ISLAE can be solved by iterations.

As an important example, we discuss the detailed description of the GMSV for an arbitrary configuration of non-overlapping partially reactive spherical sinks.

As an application of the method, we obtain the Green function that is the key ingredient to determine various characteristics of stationary diffusion such as reaction rate, escape probability, harmonic measure, residence time, and mean first passage time, to name but a few. The relevant aspects of the numerical implementation and potential applications in chemical physics, heat transfer, electrostatics, and hydrodynamics are discussed.