diffusion-fundamentals

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

Boundary-Value Problems for the Diffusion Equation in Domains with Disconnected Boundary

Sergey D. Traytak

Institute of Applied Mechanics RAS, 32-a Lenin Av., Moscow 117334, Russia, E-Mail: sergtray@mail.ru

1. Introduction

It is well known that diffusion of particles outside the trapping regions is germane to many problems in different divisions of physics and chemistry. Note also that mathematically similar problems arise in Stokes hydrodynamics, acoustics, heat transfer and electrostatics. The aim of the present paper is an attempt to give a comprehensive analysis of the different analytical approaches to the solution of the boundary-value problems for diffusion in domains with boundaries, which have complicated shapes.

2. Statement of the problem and results

For the sake of simplicity consider here the case of external mixed Dirichlet-Neumann boundary-value problem (BVP) for the steady state diffusion equation, i.e.:

$$\nabla^2 u = 0 \text{ in } \Omega^* . \qquad (1)$$

Suppose that the following boundary conditions are posed

$$u\big|_{\partial\Omega_i^D} = \varphi_i(\mathbf{x}),\ \mathbf{x} \in \partial\Omega_D,\ i = \overline{1, N_1}; \qquad (2)$$

$$\mathbf{n}_k^N \cdot \nabla u\big|_{\partial\Omega_k^N} = \chi_k(\mathbf{x}),\ \mathbf{x} \in \partial\Omega_N,\ k = \overline{1, N_2}; \qquad (3)$$

where $\varphi_i(\mathbf{x}) \in C(\partial\Omega_D)$, $\chi_k(\mathbf{x}) \in C(\partial\Omega_N)$, $\mathbf{n}_k^N$ are the unit normals to the corresponding Neumann conditions support and assume the regularity condition at infinity

$$u\big|_{r_j \to \infty} \to 0,\ j = \overline{1, N}. \qquad (4)$$

Here $\Omega^* = \mathbf{R}^3 \setminus \overline{\Omega}$, $\Omega = \Omega_D \cup \Omega_N$, $\partial\Omega^* = \partial\Omega_D \cup \partial\Omega_N$, and $\partial\Omega_D = \bigcup_{i=1}^{N_1} \partial\Omega_i^D$, $\partial\Omega_N = \bigcup_{k=1}^{N_2} \partial\Omega_k^N$ are supports of the Dirichlet and Neumann boundary conditions, respectively; u is the local concentration of the diffusive particles; $\Omega_j^{D(N)}$ are nonoverlapping continuums with smooth boundaries $\partial\Omega_j^{D(N)}$ ($j = \overline{1, N}$), $N = N_1 + N_2$.

In $3D$ only for two spheres there is an exact solution to (1)-(4) based on bispherical coordinates mapping $g : \Omega^* \to V$, (where $V \subset \mathbf{R}^3$ is an open parallelepiped) which possesses one chart atlas for the manifold Ω^*.

In more general case when $\partial\Omega_j^{D(N)}$ are the level surfaces of separable coordinates for eq. (1) the direct method of solution consist of: (a) separation of variables in local coordinate systems and (b) using appropriate addition theorems [1]. With the aid of corresponding addition theorems one can reduce the posed mixed BVP to an infinite set of linear equations (ISLE) for unknown coefficients.

It was shown that iterative solution of the obtained ISLE leads to the same series as the well-known method of reflections. We proved sufficient and necessary conditions when the reflections method is convergent [2]. Moreover we show that the classical method of images (widely used for different problems with spherical particles in electrostatics, hydrodynamics, heat and mass transfer etc.) is a special case of the method of reflections which allows us to find the solution to the Dirichlet BVP without knowledge of addition theorems. The method of images essentially uses the invariance under Kelvin transformation and so it is applicable in case of BVP for Laplace's equation only.

We also discuss the connection between addition theorems for solid spherical harmonics written in terms of spherical coordinates and Cartesian irreducible tensors. It was shown that the translation addition theorem for solid spherical harmonics is a corollary of known Hobson theorem. We apply the Cartesian irreducible tensors to solve eqs. (1)-(4) and to show that the so-called method of induced forces leads to the same ISLE in the original space.

There are several approaches to the solution of the BVP (1)-(4) in case of arbitrary smooth boundaries. Most of these methods are reduced to the relevant set of Fredholm integral equations (SFIE) of the I and II kinds. With the help of known partial Green's functions for the Dirichlet (Neumann) problem in $\Omega_j^* = \mathbf{R}^3 \setminus \bar{\Omega}_j^{D(N)}$ the original BVP may be reduced to a SFIE of the II kind. In the case of spherical boundaries with the help of multipole expansion of the fundamental solution this SFIE may be reduced to an ISLE. Using the basic theorem about representation of harmonic functions we derived the SFIE of the I kind with respect to the local fluxes into sinks $\Omega_j^{D(N)}$. In its turn we reduced the obtained set of integral equations to the corresponding ISLE. We also derived the relevant ISLE in the case when one looks for the solution of the BVP as a sum of single layer potentials. It is important to note that solution of the SFIE of the I kind is a typical ill-posed problem. Particularly for the Dirichlet boundary conditions one can show that the desired solution exists if and only if the corresponding double potential with $\varphi_i(\mathbf{x})$ as its density possesses a continuous normal derivative from both sides of the boundary $\partial\Omega^*$. It was pointed out that the Cukier-Freed method reduces the posed BVP to the solution of rather cumbersome SFIE.

References

[1] S. D. Traytak, Doctoral thesis (2005) (in Russian).

[2] S. D. Traytak, Physica A (2005) (in press).