INTRODUCTION TO THE NETWORK APPROXIMATION METHOD FOR MATERIALS MODELING

In recent years the traditional subject of continuum mechanics has grown rapidly and many new techniques have emerged. This text provides a rigorous, yet accessible introduction to the basic concepts of the network approximation method and provides a unified approach for solving a wide variety of applied problems.

As a unifying theme, the authors discuss in detail the transport problem in a system of bodies. They solve the problem of closely placed bodies using the new method of the network approximation for partial differential equations with discontinuous coefficients.

Intended for graduate students in applied mathematics and related fields such as physics, chemistry and engineering, the book is also a useful overview of the topic for researchers in these areas.

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Introduction to the Network Approximation Method for Materials Modeling

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"To my mother and great supporter, Mayya Berlyand".
L. Berlyand

"With fond memories of my wonderful time at Penn State".
A. Kolpakov

"To my mother".
A. Novikov

Contents

Preface

In the natural sciences, there exist two main classes of models – continuum and discrete. The continuum models represent media occupying a volume in space and they are described by real-valued functions of spatial variables. The discrete models correspond to systems with a finite number of components and they are described by real-valued functions of discrete variables. Typically, continuum models are based on partial differential equations whereas discrete models are described by systems of algebraic equations (or systems of ordinary differential equations for evolutionary problems).

The main objective of this book is to indicate physical phenomena and specific properties of solutions of continuum boundary-value problems, which make it possible to describe them by discrete models based on the so-called *structural* approximation. We now briefly outline the idea of this approximation and its advantages in qualitative and quantitative analysis of particle-filled composites, which are widely used in modern technology.

Compare two types of discrete approximation: a numerical approximation and a structural approximation. Here the numerical approximation means the finite-difference, finite-element and similar approximations of the original continuum problem (partial differential equation), where the discretization scale (mesh size) is adjustable depending on the desired precision.

The structural approximation is that which is based on a "physical discretization", when edges and vertices of the discrete network correspond to material objects (e.g., particles in particle-filled composites or beams in a framework). In particular, in the structural approximation the scale of discretization is determined by a natural scale representing the size of inhomogeneities (e.g., particle size). For a wide class of problems, such a structural approximation leads to discrete (finite-dimensional) *network* (graph) models.

We now present a well-known example from structural engineering to illustrate the advantages of structural discretization. Consider a framework, which consists of a finite number of beams (like a framework of a building or a bridge). Each beam is described by an ordinary differential equation whose solution contains unknown constants. The boundary conditions at the junctions of the beams provide a finite system of linear algebraic equations for these constants. This algebraic system corresponds to the structural discretization of the framework.

In contrast, let us now apply a numerical discretization to the same problem. It is possible (and, in fact, would be more accurate) to consider this framework as a system of thin continuum elements. Then we can write the corresponding partial differential equations of elasticity theory for each element (beam) and carry out a numerical discretization for the system of elements. As a result, we obtain another discrete model. While this model looks more precise, its solution requires resolving a very large system of algebraic equations with an ill-conditioned matrix (the ill-conditioning is a result of the small thickness of the structural elements), which leads to significant computational difficulties. The structural discretization in this example results in an algebraic system of much smaller dimension and solves the problem of the framework of beams with high accuracy.

In the above example the structural discretization is clearly better than the numerical discretization. However, there are many problems where a numerical approximation works very well. For example, the numerical discretization obviously must be used in the analysis of the stress–strain state in the joints of a framework of a bridge.

Another well-known example of the structural approximation is the "spring" model used to describe a great variety of phenomena from molecular dynamics to composite materials. This model became classical after the book by M. Born and K. Huang (1954) and has been intensively used ever since.

The two models mentioned above, belonging to the same class of structural models, demonstrate the strong difference in their justification. The finite-dimensional model of a framework is a model at the mathematical level of rigor. At the same time, "spring" models are usually considered as "the physical level of rigor" models, which can be used to describe the corresponding phenomenon qualitatively but not quantitatively.

Structural models are naturally related to graphs (networks) describing relations between the interacting elements of the system under consideration. This is why they are often referred to as *network* models.

Various network models have been widely used in the physics and engineering literature for the construction of simplified analogs of continuum problems. Such analogs are usually obtained based on some kind of an intuitive consideration, and the relation between the original continuum model and the corresponding network is not derived in any systematic way. The problem of the approximation of a given continuum model by a corresponding discrete network has received far less attention. Here by approximation we mean a rigorous justification of the "closeness" in some sense (e.g., asymptotically) between two models with a controlled error estimate. Such justification includes a systematic theoretical derivation of a network from a given continuum model. The approximation issue plays a crucial role in determining the limits of validity of network models. If the issue of validity is not addressed, then a network model may not approximate the continuum problem and therefore may provide misleading results.

The specific feature of the problems presented in this book is that the mathematical methods are intimately related to physical phenomena and the development of our mathematical approach and the analysis of specific problems for various particle-filled composites is done hand in hand. This feature determines our style of presentation, which is a unity of mathematics and applications. Since typically the number of particles is large, the study of particle-filled composites involves large-scale networks. As a result, we face the specific issues of large networks, such as percolation and homogenization.

The problem considered in this book is described by simple constitutive laws (Ohm's, Stokes', Fourier's) which correspond to well-known linear equations. The main difficulty is due to the complex geometry of the domain where these equations are considered. This geometry includes the shape of particles, non-periodicity of the particle locations and close to maximal concentration.

A number of recent results available only in journal publications are treated within the framework of this approach, which makes it convenient for the reader.

This book is an introduction to a wide and dynamically developed field of applied mathematics. Its aim is to present, simultaneously with mathematical rigor and in the simplest possible way, the basic concepts of the network approximation method. For this reason, the authors have selected for detailed exposition one of the existing approaches to developing the network approximation (which can be characterized as the direct construction of trial functions providing asymptotically exact two-sided estimates) and one example of the application of the network approximation method to a real-world problem (computation of the transport property of a disordered high-contrast high-filled composite, including the solution of the well-known problem of the influence of polydispersity on the transport property of the composites).

The authors restrict the presentation to a two-dimensional problem and bodies, which have the shape of circular disks. The reason for this restriction is that this is the modern state of network approximation theory. For example, in this case the network approximation is developed not only for a finite number of bodies but also for an infinite number of bodies (the homogenization type network approximation). Some applied results were obtained by using the method of complex variables. The modern state of the general framework of approximation theory (the theory for arbitrary dimensions and bodies of arbitrary shape) can be characterized as a *work in progress*. Significant progress has been made in some directions in these fields. At the same time, some problems resolved for the two-dimensional problem and bodies, which have the shape of circular disks, remain open in the general case. So, the most complete theory of the network approximation now exists for the particular case described above. The authors decided to write an introduction to the network approximation using this particular problem rather than wait for the completion of investigations of the general case.

The structure of the book is the following:

– Chapter 1 contains a review of mathematical notions used in the analysis of transport problems in composite materials.
– Chapter 2 contains the formulation of the problem and its brief history.
– Chapter 3 presents the network approximation method for linear problems in the presence of a finite number of inclusions.
– Chapter 4 discusses polydispersed composites. This illustrates how the network approximation method is used for the solution of applied problems.
– Chapter 5 expands the network approximation method to an infinite system of disks.
– Chapter 6 expands the network approximation method to the nonlinear problem. We use this chapter also to demonstrate an approach to the construction of a network approximation based on the idea of a perforated medium.
– Chapter 7 demonstrates that the network model provides us with an approximation not only for overall characteristics (such as the total flux, energy) but nodal values approximate potentials of inclusions.
– Chapter 8 presents some results on the conductivity of polydispersed materials obtained by using the method of variables complex.

This book is intended for graduate students in applied mathematics, materials science, physics, mechanics, chemistry and engineering as an introduction to the mathematically rigorous theory of network approximations for partial differential problems or, alternatively, the theory of network models for continuum problems. The prospective applications of network approximation theory could be of interest to industrial engineers, who design composite materials, suspensions, powders, etc.

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The authors offer this book in the hope that it may prove useful to researchers, professors and students working in the areas of pure and applied mathematics, physics, chemistry and material science, especially dealing with problems accounting for spatial inhomogeneity.

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