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Influence graphs and the generalized finite difference method

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Abstract

This paper introduces directed graphs on which the evolution of a physical quantity depends only on local neighborhoods. These graphs are then used to model transfer phenomena occurring under a convective mode or a diffusive mode. The conditions under which the state associated to such graphs approaches the solution of a diffusion-convection partial differential model are established. An algorithm permitting to determine consistent neighborhoods is described and recognized as a generalization of the finite difference method. Examples of application are presented in order to illustrate the practical applicability of these concepts.

Keywords: Discrete mechanics; Generalized finite differences; Meshless methods

1. Introduction

Transfer phenomena are usually modeled under the mathematical framework of continuous fields, leading to partial differential equations. These equations are either investigated directly by analytical methods or are discretized into a finite set of algebraic relations involving discrete values in order to proceed to numerical simulations based on various mathematical approximations (finite differences, finite volumes, finite elements, boundary elements, etc.). Taking an alternate path, one may also directly formulate the laws of evolution for a discrete system and search for the necessary conditions under which this discrete system will behave more and more as the continuous one, as the number of its individual components increases inside a domain of a given shape. Examples of this approach may be found in [1] concerning particle flows, in [2] for elastic deformations, or in [3] for the case of electromagnetism. Flows governed by Navier–Stokes equations have been simulated by colliding particles on lattices of nodes [4] and convergence results have been obtained for lattices associated with a sufficient degree of rotational symmetry.

Section 2 of the present paper will be devoted to the description of a set of nodes on which a quantity u_i evolves under the influence of the values u_j recorded on the neighboring nodes. Section 3 will introduce the conditions allowing this set to approach more and more closely the behavior of a continuum as it is made finer and finer inside a given region of space. Assuming these conditions are verified, the discrete state approaches in the limit the solution of a diffusion/convection partial differential equation. From this point of view, this framework may also be considered as a means to generalize the finite difference schemes on a set of nodes freely distributed in a given domain (see Figs. 8 and 10).

The second part of this work describes a practical way to use the conditions of consistency in order to set up the approximating differential systems. Extensive work was applied previously in the search to properly extend the kingdom of the finite difference method outside the regions of orthogonal grids. Early works date back as far as [5] or [6], and similar attempts appeared from time to time in the literature as an effort to compete with the ever dominating finite element method. Jensen [7] used a Taylor expansion written on a set of user-defined neighboring nodes (“The word neighbor is loosely used in this context to mean *nearby*”) to replace the partial derivatives by a combination

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of unknown values, but soon realized that the matrices obtained are generally singular when the neighbors are selected on a sole distance criterion. In that case, the choice of neighbors must be modified but "this feature was not yet incorporated in the computations". In order to alleviate this difficulty, Perrone and Kao [8] partitioned the space around the central node into eight sectors in which to select five neighbors on the basis of distance to the center. This strategy, although clearly improving on the past, did not fully succeed as the authors conclude that there were "two key factors: (a) avoidance of a singularity problem in matrix A; (b) ability to obtain good derivative approximations...". The first general purpose program successfully written for irregular grids seems to be the FIDAM code described in [9] and applied to solve various problems in mechanics. Let us summarize the work of these pioneers: on a central node (x_0, y_0), five unknown derivatives have to be computed from the values obtained on the others nodes. A subset of eight or more nodes is selected near the central node in all four quadrants and is globally called the *star*. These nodes are then weighed (the nearer the node the larger the weight) and the L_2 norm of the residual of five linear equations involving the five unknowns is then minimized. The four key features addressed by subsequent works on this same subject appear in this paper: a. How many nodes to include in the stars? (b) How to select these nodes? (c) What weighting function to use? (d) How to justify the use of a least-squares approximation of a Taylor formula? Only the last of these questions has led to a definitive answer by identifying in this approach a moving least-squares interpolation method (MLS [10]), related afterwards to some local variational principles giving way to the so-called meshless methods [11–13]. Following these works, the mainstream of research dealt with the variational framework either as a local finite element method (partition of unity methods [14]) or as a variation of a kernel-based approach (e.g. the smoothed particle method [15]).

However, in the author's opinion, none of these various methods (as successful as they may be) can be considered as a *bona fide* generalization of this old lady, the finite difference method, on the basis of at least three strong points. Firstly, a finite difference solution is not a function but a set of discrete values (the fact that continuous objects *could* be interpolated from this set is irrelevant), and a strict distinction should be maintained between external (Taylor expansion) and internal (weak formulation) methods. Secondly, in a finite difference method, the Taylor expansion must be exactly verified by the discrete values up to a predetermined order, and not as best as it can be. And, last but not least, a true generalization should result in the usual tight and efficient schemes when applied to the same orthogonal grids. Let us recall here that four neighbors (i.e. five points schemes) suffice to approximate a Laplacian up to the order two (this is not so bad when compared to the classical serendipity quadrilateral finite element scheme which needs up to 20 neighbors to achieve the same order of convergence on the same grid). This is not the case for any of the preceding methods, some of them demanding to include up to 40 neighbors in each star to ensure well-conditioned matrices and convergence of results, without any regard to the spatial distribution of nodes.

The description and study of the influence graphs done in Sections 2 and 3 placed in our hands a tool to recognize if a graph approximates a continuum consistently or not, but do not provide a direct way to construct consistent graphs. In Section 4, an algorithm will be described to accomplish that task, providing a first set (probably not unique) of answers to questions (a) and (b). This algorithm does not make use of any weighting function and, there, question c. finds its extinction. In short, the answer to (a) and (b) is simply: don't decide (how many and where) for the algorithm. Let it find itself. Give it your own preferences: tight and few populated schemes. These preferences will be taken into account only when a solution must be selected from many possibilities. For orthogonal grids, there is no choice: the usual schemes are the only ones brought out by the computations. The main features of this generalized finite difference method will be illustrated in Section 6 that describes three examples of application in the field of diffusive and convective transfer.

2. Influence graphs

Let us denote by $\mathbf{N} = \{P_i\}$ a set of N fixed points of $\mathbb{R}^d$. These points are the *nodes* of the graph. The location of node i is given by $\mathbf{X}_i$. A node is connected to some other nodes (which are called its neighbors) by a set of *directed edges*, defined as a couple (P_i, P_j) of nodes. The set of edges $\mathbf{E}$ is a subset of the Cartesian product $\mathbf{N} \times \mathbf{N}$. The whole topological graph $\mathbf{G}$ is given by the couple $(\mathbf{N}, \mathbf{E})$, with $N = \mathrm{card}(\mathbf{N})$ and $N_e = \mathrm{card}(\mathbf{E})$. An index p is assigned to each edge $(i \xrightarrow{p} j)$. To node P_i is associated the set $I_e(i)$ collecting all the edges issued from i

$$I_e(i) = \{p \,|\, (i \xrightarrow{p} j)\}. \tag{1}$$

Let be a node i, an edge $p \in I_e(i)$ and two scalar values (u_i, u_j) given on the nodes (P_i, P_j). We introduce the following notations (see Fig. 1):

$$\ell_p = \|\mathbf{X}_j - \mathbf{X}_i\|, \quad \mathbf{S}_p = \big(\mathbf{X}_j - \mathbf{X}_i\big)/\ell_p,$$
$$u^p = u_j - u_i, \quad a_i^p = j. \tag{2}$$

The vectors $\mathbf{S}_p$ are called the *directors* of the graph $\mathbf{G}$.

The quantity u_i evolves under the influence of the neighboring values. Let us view edge $p \in I_e(i)$ as a sensor continuously reading the value u_j. These values are accumulated by a controller which issues a command C_i to the node i. This command causes a variation of $u_i(t)$ according to the law $\mu_i \, \mathrm{d}u_i/\mathrm{d}t = C_i$, where μ_i is a positive real number (the inertia of i) associated to node i. The command C_i is the sum of three terms: the first term is a local source