TOWARDS A METHOD TO GENERALLY DESCRIBE PHYSICAL SPATIAL PROCESSES

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Abstract: Spatial processes are the focus of geography and should play a prominent role in geographic information systems (GIS). However, current GIS focus on the static description of properties in space and do not systematically support processes. A general method to describe spatial processes is a prerequisite to including processes in GIS software. This paper outlines an attempt to a general and application independent method to describe processes, limited currently to physical spatial processes. The methodology is based on first modeling a process with a deterministic model. The deterministic models employed here divide the region of interest into blocks and define the influence of the process on each block. The resulting model equations are then related to partial differential equations (PDEs), which are an alternative method for describing processes. Thereby, the qualitative characteristics of processes are identified. A method for describing processes has to be capable of covering the identified characteristics of the processes. As an example the process of diffusion of a contaminant in water is analyzed. The results of this study suggest that this approach allows identifying commonalities among spatial physical processes. These insights can lead to a set of types of processes on which a method to describe spatial processes can be based in the long run.

Keywords: spatial physical processes, deterministic models, partial differential equations

1. INTRODUCTION

Most currently available models of space in geographic information systems (GIS) focus on the representation of the earth in a static way; there is, however, an increasing need to systematically support change, dynamics, and processes in GIS, representations of data, visualization schemes, etc. (MacEachren 1995; Frank 1998; Blok 2000; Yuan 2001; Miller and Wentz 2003; Worboys 2005; Goodchild et al. 2007).

Spatial processes are processes taking place in space and may depend on location in space. They show different natures and are studied in different disciplines like ecology, geography, geocomputation, and physics. Examples are the spread of forest fires (Yuan 2001), the growth of cities (Batty et al. 1999), the migration of species (Seppelt 2005), and the flow of water (Mitasova and Mitas 2002). Terminology across disciplines varies. Different disciplines describe the process of interest in the application, but no commonality between disciplines is achieved.

Physical spatial processes are governed by physical laws like mass conservation. In addition, they are continuous processes and are dominated by local influences. They are considered spatial, if they fall into the temporal and spatial frequency interval typical for geography.

The long term goal of the work reported here is to provide the outline of a domain and application independent method to generally describe spatial processes, limited to physical spatial processes. Such a method is a prerequisite to including processes in GIS software and to extending our current concepts of space.

For describing physical spatial processes on a general level, we need to identify the qualitative characteristics, which explain the behavior of the process over time. Our methodology is based on modeling a spatial process with two different models, namely deterministic block models and partial differential equation (PDE) models. These two types of models are alternative ways to describe processes, having different advantages. Block models of processes are useful for conceptualizing processes and for simulating processes computationally. Models of processes based on PDEs are useful for identifying generic properties of a process or a family of processes. The theory of linear PDEs discerns three main types of processes that are described by different types of equations: wave-like, diffusion-like, and steady-state processes.

Deterministic models formulated as difference equations can be related to PDEs. Thereby we establish a link between the two models and have a description of a process from both points of view. This procedure allows us to gather information about qualitative characteristics of a process, which have to be included in the description of a process. This methodology is applied here, as a practical example, to the process of the diffusion of a contaminant in water.

The results of our research show that general insights on a formal and qualitative level can be gained. Applying the approach repeatedly on a list of spatial physical processes will allow the identification of commonalities among processes. This is an important step towards a set of tools for describing spatial physical processes.

This article is divided into seven sections. Following the introduction, a brief review of the literature related to spatial processes and GIS is given. Subsequent to a definition of spatial physical processes in section 3, two models for these processes are introduced: deterministic models and PDEs. A specific example of modeling a process is given in section 5 and the characteristics of the example process discussed in section 6. The section on conclusions and future work is the final section of the paper.

2. SPATIAL PROCESSES AND GEOGRAPHIC INFORMATION SYSTEMS

Numerous attempts to describe spatial processes exist. In the sequel of the quantitative revolution in geography a focus on detailed treatment of processes in geography became feasible. Abler, Adams, and Gould (1977, p.60) define spatial processes as "…mechanisms which produce the spatial structures of distributions". For them the task of geography is to answer the question: "why are spatial distributions structured the way they are?" (Abler et al. 1977, p.56). Getis and Boots (1978) and Cliff and Ord (1981) worked in this direction. They were interested in understanding the connection between a process and the resulting form of patterns on a map. They intended to connect the static, observable state of geographic space with the process that shaped the geographic reality, linking the snapshot with the dynamics.

The work on spatial processes in the field of geographic information systems and science is extensive and can be driven by very different objectives. The following listing briefly mentions various related achievements and research contributions:

- Development of software packages like Map Algebra (Tomlin 1990) and PCRaster (Van Deursen 1995) for analyzing and simulating spatial phenomena.

- Development or extension of data models for handling the dynamics or particularities like continuity of spatial phenomena (Kemp 1992; Reitsma and Albrecht 2005; Worboys 2005; Goodchild et al. 2007).
- Analysis of analytical GIS operations and investigation of the links between processes manipulating GIS data and processes in reality (Albrecht 1998).
- Investigation of the linkage of modeling tools and GIS (Kemp 1992; Van Deursen 1995; Abel et al. 1997; Hornsby and Egenhofer 1997; Bivand and Lucas 2000).
- Investigation of a single process like diffusion (Hornsby 1996) or geographic movement (Tobler 1981).
- Investigation of network geography and the representation of network related process in GIS (Batty 2005).
- Modeling of geographic phenomena with existing respectively prototype GI systems (Yuan 2001; Mitasova and Mitas 2002).

Despite all the efforts to analyzing and classifying spatial processes, these have not been widely accepted yet. Part of the confusion, making discussion of processes so difficult, is the sheer variability. The scope of the discussion is overwhelming and grouping in arbitrary many ways possible. The paper addresses this issue by aiming at a domain and application independent method of analyzing physical spatial processes. The novel contribution of this work is the use of PDEs and deterministic models in a qualitative study of spatial processes.

3. WHAT ARE PHYSICAL SPATIAL PROCESSES

Generally speaking, spatial processes happen in space and may depend on location in space. Getis and Boots (1978, p.1) define spatial processes as "…tendencies for elements to come together in space (agglomeration) or to spread in space (diffusion)". These definitions indicate that nearly every spatial phenomenon is a process and discussing processes seems to be discussing everything.

In order to avoid this trap, the approach here concentrates first on physical processes. This links to the tiered ontology Frank (2001) has used in other contexts successfully: physical processes cover a very large part of geographic processes, but not all of them. If this restriction is useful it must lead to conceptual clarity and extending some of the insight beyond the limitation possible.

Ontologically we separate the physical reality as the part of reality which is governed by physical laws from the tier of our reality which is socially constructed and governed by social (legal) rules. Ontologists assume that physical processes have all their effects continuously in space and their influences restricted to the neighborhood. Therefore, physical processes are strictly local and do not depend on global knowledge. Frank (2001) pointed out that physical processes are describable by (partial) differential equations.

This argument is used here in the reverse direction: the physical processes studied here are exactly those describable by differential equations; this restriction enforces the focus on strictly local processes. This restriction seems to be acceptable in geography; Tobler's first law of geography says: "everything is related to everything else, but near things are more related than distant things" (Tobler 1970, p.236).

Processes are considered geographic if their frequency in time or space falls into the frequency interval typical for geography. Geography focuses on spatial objects of size between 0.1m and 40.000km and processes where change is noticeable in minutes to 10.000 years. Typical examples for geographic physical processes include: soil erosion, migration, groundwater flow, stream flow, sediment transport, forest fires, floods, saltwater intrusion, surface runoff, flux of pesticides.

Excluded as non physical are processes which are not controlled by physical causation, but by information causation (Frank 2007). If a computerized or human information processing unit at one place is the cause of a physical spatial process at a possibly distant other place, we speak of information causation. Information causation is not limited to neighborhood: a decision by a single person in a "center of power" can be transmitted for and have devastating effects at a very distant location. Such information caused processes are excluded from the current discussion.

4. TWO MODELS OF SPATIAL PHYSICAL PROCESSES

Two fully general and equivalent models for the description of spatial physical processes are presented in this section: deterministic models based on blocks and partial differential equation (PDE) models. The block model describes the process and its characteristics with respect to blocks of finite size. These models are useful for conceptualizations of processes and communication about processes but also a useful approach to computational simulation. The theoretical analysis of physical spatial processes is helped by the focus on making the blocks smaller and smaller till they become infinitely small; this leads to continuous models of processes, which are here represented by partial differential equations. The two models are equivalent and every process can be described in either of them and the translation between the two models is always possible.

4.1. Deterministic Models Based on Blocks

An important principle of physical systems is the conservation of some quantity like mass or energy. Fundamental conservation laws state, that the amounts of a quantity going in, going out, and being created or destroyed in a region, have to correspond to the amount of change in a certain region (Logan 2004). Besides these laws of conservation that describe the storage of a quantity, the transfer of a quantity is described by transport laws or flow laws (Thomas and Huggett 1980). Thomas and Huggett (1980, p.64) define a deterministic model as "a storage equation in which the input and output rates are defined by suitable transport laws." The following explanations of deterministic models are based on (Thomas and Huggett 1980).

A physical spatial process occurs in space and we can cut out a small piece of space, a block or an element, and describe the change in the relevant parameters describing the process. We thereby define the spatial domain as a set of blocks (Fig. 1(a)). Blocks can be combined in various ways, depending on the process; for studying, e.g., water flow in a river, blocks may be arranged in a line (Fig. 1(b)).

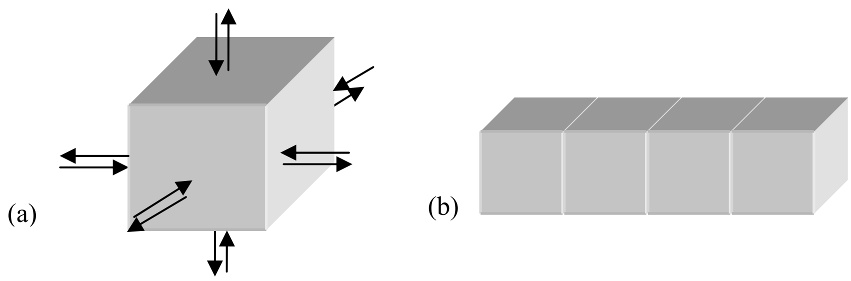

Fig. 1. (a) a block as spatial unit, (b) a sequential alignment of blocks for studying for example water flow in a river.

After selecting the process of interest and defining the spatial domain, storage equations are established for every block in the spatial domain. As said above, the storage equations state the change of a quantity Δq in the block; this change is determined by the difference of the flow in f_i and the flow out f_o of the block in a given time interval Δt (see Eq. 4.1.1).

$$\Delta q = \left(f_i - f_o \right) \Delta t \tag{4.1.1}$$

For defining the input and output terms of the quantity, we need transport laws. These laws are derived from physical characteristics of the processes. Conservation laws apply again, which means that the outflow of a block through one face must be equal to the inflow in the neighboring block. Important transport laws are Fick's first law of diffusion, Fourier's law of heat transport, and Darcy's law of water flow. Fick's law, for example, states that the negative gradient of the concentration of the quantity (ΔC) times the diffusion coefficient D of the quantity, is proportional to the quantity flow rate f . Eq. 4.1.2 states the gradient of the concentration of a quantity in x direction with $\frac{\Delta C}{\Delta x}$.

$$f = D\left(-\frac{\Delta C}{\Delta x} \right) \tag{4.1.2}$$

The transport law applies to all blocks except those at the boundary of the region of interest. Special flow conditions known as boundary conditions are defined for blocks at the region's boundary.

The equations that are formed by applying this modeling technique describe the storage change in discrete time intervals t1, t2, t3 etc. Therefore, they are difference equations. In a difference equation the change of a quantity over time can be expressed by the relation between successive values of the quantity. For running the models, initial conditions for the storages at the start, boundary conditions and parameter values have to be given. The difference equations can then be solved, the results evaluated and the model adjusted.

4.2. Differential Equations to Model Processes

A differential equation is an equation where variables and derivations from variables are brought into a relation. The general solution to a differential equation is a function or a family of functions describing some aspect of a process. Ordinary differential equations (ODEs) depend on one independent variable and contain derivatives with respect to this variable only.

Spatial processes are described by partial differential equations (PDEs), because they depend on more than one independent variable like space and time, or several spatial dimensions. PDEs allow modeling the change of a variable of interest that depends on more than one independent variable

(Logan 2004); the derivatives in PDEs are partial in the independent variables.

Partial differential equations (PDEs) have long been used for modeling, analyzing, and simulating continuous physical phenomena as well as spatial phenomena (Tobler 1981; Giudici 2002; Mitasova and Mitas 2002). PDEs are widely applicable, because they show how processes evolve.

In this paper, PDEs are used for describing generic or theoretical information about spatial processes. Theoretical characteristics of PDEs are therefore more important here than computational issues related to PDEs. The focus is on basic, linear PDEs of at most third order. In the theory on PDEs, three main types of processes are differentiated: wave-like, diffusion-like, and steady-state processes. Different equations are used for describing these types of processes. The following specifications of the types of processes are based on (Logan 2004).

The types of equations used for modeling *wave-like processes*, are hyperbolic PDEs. These equations are evolution equations and model how a process evolves over time. One example for a wave-like process is advection or convection. The advection process describes the bulk movement of particles in some transporting medium like water or air. A boat floating downstream in a river is an example for an advection process.

Diffusion-like processes are modeled with parabolic equations, which are evolution equations like the hyperbolic equations. Diffusion describes the random motion of particles, which generally diffuse from regions with a higher to regions with a lower concentration of particles. The example of a contaminant diffusing in water is discussed in section 5 of this paper.

In the case of a *steady-state process*, we deal with an elliptic equation. These types of equations do not contain a time variable and are therefore independent of time. They are known as equilibrium equations that model processes like the steady-state flow in fields where a balance between input and output in the systems exists. An example for a steady-state process is the flow of groundwater in a certain region with fixed boundary conditions.

An important difference between wave-like and diffusion-like processes is how the quantity of interest is affected over time. Wave-like processes preserve the quantity, whereas diffusion-like processes tend to smear out the initial configuration of the quantity. Wave-like and diffusion-like phenomena are two important types of phenomena that occur in different disciplines. Combinations of these two types of motions are also possible (Table 1).

An important part of the methodology in this work is relating difference equations to PDEs and thereby deriving theoretical insights about a process. For this purpose, a list of linear PDEs was compiled based on (Hohage

2004; Logan 2004; Markowich 2007). The recurrence of equations in the different sources suggests that it gives an overview of basic linear PDEs, although the list may not be complete.

Table 1. Linear PDEs assigned to the three main types of processes

Types of phenomena	Type of equation	PDEs
Wave-like phenomena	Hyperbolic	
		Wave equation
		Advection equation
		Advection-decay equation
		McKendrick or von Foerster equation
		Continuity equation
		Boltzmann equation
Diffusion-like phenomena	Parabolic	
		Heat equation
		Diffusion equation
		Diffusion-decay equation/ Diffusion-growth equation
		Advection-diffusion equation
		Advection-diffusion-decay equation
		Continuity equation
Steady-state phenomena	Elliptic	
		Poisson's equation
		Laplace's equation
		Helmholtz equation

5. EXAMPLE: DIFFUSION OF A CONTAMINANT IN WATER

The two types of mathematical models introduced in the previous section, are now applied to the specific example of the diffusion of a contaminant in water. Section 5.1 gives the deterministic block model of the process as difference equations. This block model provides a conceptualization of the process. In section 5.2 the difference equations are related to the corresponding partial differential equation, which sheds more light on generic properties of the process. The insights about the example process are discussed in section 6.

5.1. A Block Model of the Example Process

The derivation of the conceptual deterministic model of the diffusion of a contaminant in water is based on examples discussed in (Thomas and Huggett 1980). We assume that the diffusion of a contaminant follows the law of mass conservation. Fick's law of diffusion defines the rate at which the contaminant diffuses along the contaminant concentration gradient.

The spatial domain in which the process takes place is an enclosed and stationary water body like a basin. We divide the water body into a set of blocks that are placed one next to another and also one above and below another. The following storage equation is formulated for a block surrounded by other blocks at all of its six faces. The contaminant can enter the block of interest from any of its six faces. There is a certain amount of the contaminant in the water body, which is conserved under the law of mass conservation, and no sources or sinks of contaminants exist in this example. The symbols used in the following equations are:

C … concentration of the contaminant
D … contaminant diffusion coefficient
A … area of a face of the block
V … volume of a block
f … flow rate due to diffusion
f_i … contaminant inflow in a block
f_o … contaminant outflow of a block
Δ … a difference
Δq … change in contaminant storage in a block in a time interval
Δt … time interval
Δx … distance interval in x direction
Δy … distance interval in y direction
Δz … distance interval in z direction

The change of the contaminant storage in a block of water over a time interval is specified by the following equation (Eq. 5.1.1):

$$\Delta q = \left(f_i - f_o \right) A \, \Delta t \tag{5.1.1}$$

The input and output of the contaminant are due to diffusion, which is the "movement of [the contaminant] along the concentration gradient between two blocks" (Thomas and Huggett 1980, p.119). Fick's law defines the flow rate in the case of diffusion as "proportional to the negative gradient of [contaminant concentration] through the face of the block" (Thomas and Huggett 1980, p.119). Eq. 5.1.2 states the flow rate in all directions of a block.

$$f = (f_i - f_o) = D\left(-\frac{\Delta C}{\Delta x}\right) + D\left(-\frac{\Delta C}{\Delta y}\right) + D\left(-\frac{\Delta C}{\Delta z}\right) \tag{5.1.2}$$

A second way of identifying the changes in the storage of the contaminant is multiplying the change in the concentration of the contaminant by the volume of the block. The change in the contaminant concentration corresponds to the difference in the contaminant concentration at the beginning and at the end of a time interval (Eq. 5.1.3).

$$\Delta q = \Delta C\ V \tag{5.1.3}$$

We equate the two equations describing the change in the storage of the contaminant (Eq. 5.1.1, Eq. 51.3), simplify them and get:

$$\frac{\Delta C}{\Delta t} = -\left[\frac{\Delta}{\Delta x}\left(-\frac{D\,\Delta C}{\Delta x}\right) + \frac{\Delta}{\Delta y}\left(-\frac{D\,\Delta C}{\Delta y}\right) + \frac{\Delta}{\Delta z}\left(-\frac{D\,\Delta C}{\Delta z}\right)\right] \tag{5.1.4}$$

Eq. 5.1.4 can be rewritten in the following way:

$$\frac{\Delta C}{\Delta t} = D\left(\frac{\Delta^2 C}{\Delta x^2} + \frac{\Delta^2 C}{\Delta y^2} + \frac{\Delta^2 C}{\Delta z^2}\right) \tag{5.1.5}$$

This difference equation (Eq. 5.1.5) describes the diffusion of a contaminant in a water basin. The conceptual model is complete with the derivation of the difference equation. For an actual simulation of the problem, parameters, initial conditions and boundary conditions would have to be specified.

5.2. Relating the Block Model to a PDE

In section 5.1 we derived a deterministic model of the process of diffusion of a contaminant in a water basin. This model is based on discrete temporal and spatial units, with the spatial units being blocks. If we imagine we make these units smaller and smaller until they are infinitely small, we can understand the difference equation as a continuous differential equation. This idea is used here for relating the deterministic model of a process to a PDE; the set of PDEs available was listed in Table 1. Usually, this procedure is used in the reverse, and continuous PDEs are approximated with difference equations to find their solution. Seen from a conceptual, rather than a mathematically precise point of view, the difference equation (Eq. 5.1.5) corresponds to the following partial differential equation (Eq. 5.2.1):

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{5.2.1}$$

This partial differential equation is known as the diffusion equation without sources in three dimensions. This equation is a second order, linear PDE. The meaning of the PDE is of course equivalent to the meaning of the difference equation derived in the previous section, but independent of the block structure assumed in section 5.1. The state variable *C(x,y,z,t)* depends on time and three spatial dimensions. It defines the concentration of the contaminant in space over time. The right hand side of the equation defines the flow of the quantity at a certain moment in time. The next section discusses the insights we gain through applying the presented methodology on the example process.

6. QUALITATIVE INSIGHTS ABOUT THE EXAMPLE PROCESS

As a physical spatial process, the process adheres to physical principles of mass conservation and Fick's law for determining the rate of diffusion. Particles always diffuse from areas with higher to those with lower concentrations of particles; if there is no difference in the concentration of particles between two blocks, no flow takes place. Expressed differently, diffusion takes place down the concentration gradient of the contaminant in water.

The modeling of the example process with difference equations, allows us to easily determine the components that make up a process. In our example we have:

- the concentration of the contaminant, which depends on time and space and is defined by the flow of the contaminant over time.
- the flow of the contaminant, which is specified by the contaminant diffusion coefficient times the negative contaminant concentration gradient across a face.

The related partial differential equation is the diffusion equation, which is a parabolic equation showing the behavior of a process over time. The behavior of the process we can expect is that the original contaminant concentration spreads throughout the cells in a random manner and gets lower in specific cells the more blocks are affected by the process. An exemplary two-dimensional representation of the behavior of this process is shown in Fig. 2.

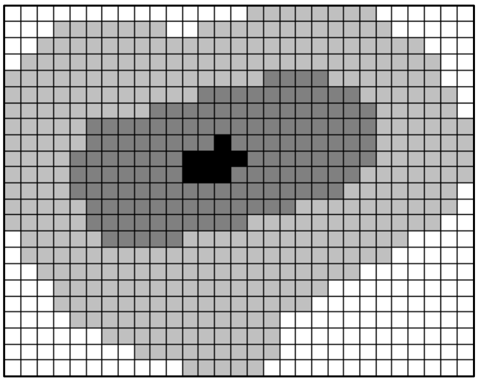

Fig. 2. Exemplary two-dimensional representation of a substance diffusing in space; the darker the color the higher the concentration of the substance.

7. CONCLUSIONS AND FUTURE WORK

In this paper we presented our approach to gaining insight in spatial physical processes on a qualitative level. We employ simple deterministic models based on blocks for modeling processes and getting conceptualizations of processes. The resulting model equations are then related to types of partial differential equations (Table 1).

The methodology was presented exemplarily for the process of contaminant diffusion in water and general properties of this process were identified. In a next step, this methodology will be applied repeatedly to different spatial physical processes; thereby a catalog of components for describing qualitative characteristics of processes will be created. This catalog will allow the domain and application independent description of physical spatial processes on a qualitative level. One characteristic of the components in the catalog has to be that they can be composed in order to form more complex processes out of basic components.

Having in mind the extension of models of space and GIS with general functionality for handling processes, such a catalog could serve the following purpose in the long term: it could serve as a toolbox for describing a process qualitatively and for generating a concept for modeling a process. Such a concept of a process model would contain the required data sets, parameters and equations describing the general behavior of a process. In the case of the example of the diffusion of a contaminant in water, the required data set is the distribution of the contaminant, which serves as initial condition. For solving the diffusion equation, the diffusion parameter and boundary conditions have to be given.

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