

# Notes on the possibilities and limitations of using topological tools in mechanical modeling of media

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**Abstract.** In the mechanical modeling of the media, the atomic-molecular structure of the material is usually neglected, furthermore, with regard to the characteristic distance of the atomic-molecular structure, the media is considered to be a continuous material distribution. Referring to the continuous distribution, we use the tools of differential and integral calculus for the mechanical-mathematical description of the media. The use of these mathematical tools has conditions and limitations: there must be a sort of topological order in the examined space. This order records the relative position of the points. The fixed position relative to each other makes it possible to describe only such mappings that retain the fixed position relative to one another. Thus, it is possible to distinguish between strain and rearrangement, and at the same time to define the boundaries of the possibilities offered by the applied mathematical tools: the continuum many points set provides the basis of the topological description for the classical continuum, a set of finite points in the grid network with its internal structural features, provides the basis of the topological description for the grid (that is generalized) continuum.

## 1. Introduction

When describing the behavior of elastic materials, the material is considered to be continuous. In the model, only the degree of displacement freedom is assigned to each point of the material considered as continuous (see e.g. [1,2]). The model can be expanded by assigning to each point of the material considered to be continuous, its rotational degree of freedom in addition to its displacement (see e.g. [3]), then we gain the micropolar theory of elasticity. The model is purely theoretical, the author [3] indicates (in fact complains) that no experimentally measured material constants can be found to the new theory. The expanded continuous media model can be further expanded to include pointers (“directors”), granules (“micro continuums”), and the rotation of directions, the strain states of granules will become the additional kinematic variables (see e.g. [4,5]).

The question arises as to whether the granules in the granular material can be attributed to a degree of distinct rotational degree of freedom that is independent of the material embedding the granule: in concrete, the gravel grain cannot rotate. It cannot rotate theoretically, because then a force independent of the cement stone has to act upon it to rotate, but we have no knowledge of such force. It cannot rotate practically because the fracture tests prove that concrete breaks in a way that gravel does not fall out of the cement stone but breaks.

The question arises as to what kind of continuous and discrete modeling is possible for materials with discrete, atomic-molecular, or larger scale internal structures [6,7,8,9]. In the depths of the research, the same question arose: in order to create a model of continuous media, the material must not only be

continuous but must also have an internal order. This order can be identified with the topological order [10]. In this paper, we review the conditions and consequences of using topological tools: continuous mapping, differential and integral calculus.

## **2. Description of the order. Consecutiveness of series and topology**

The order in the body is interpreted as the atoms and/or molecules that make up the body adjacent to one another, making them belong together. The preservation of the order can be defined as the atoms and/or molecules adjacent to each other before a visible effect remains and belong together after the external effect.

In order to “describe” the order, the space occupied by the atoms and/or molecules constituting the body is considered fixed; the location of the atoms and/or molecules is given by the reference point of each atom and/or molecule. The point network thus obtained is considered a grid. (We take the grid of rock salt crystal as an example). In the grid the order is characterized by the fact that the order of the grid points in one line along each direction is unchanged, and that each grid point can be specified by a unique triple of numbers and this unique indicator does not change during an effect upon the body.

In addition to the triple, there is another possible way to specify the order: specify the set of all the points that belong to each other. This is the well-known neighborhood system from point topology [11]. In the topology, the order in the set of points, the “interconnection” between the points is interpreted with the neighborhoods and at the same time “interconnection” is fixed for all points of the point set once and for all. In the set of points, “interconnection” means that two or more points belong to the same neighborhood. Since we determine for each point which points belong to its neighborhood, the neighborhood system, i.e. the topological order, reflects the order (consecutiveness) of the points relative to one another (see e.g. [11]).

The topological order (and topological mapping) also allows two topological spaces to be mapped while preserving the internal structure of the topological space.

The concept of topology has been developed by describing the various accumulative and separability properties of the point sequences in the metric spaces. The topological space is a “generalization” of the metric space in which the topological properties are not expressed by the metric but more general, e.g. neighborhood system. It is noteworthy that there is no need to “construct” a “rich” topological space, because a set of real numbers (obtained with metrics from the Euclidean space) already has the topological qualities needed to perform differentiation and integration (e.g. existence of accumulation points, separation of neighborhoods, or in other words the spaces of the n-tuple numbers is Hausdorff space (see e.g. [11,12] for topological spaces and analysis).

Hereinafter, the topological space refers to Hausdorff space locally.

The consequences of the topological order in the topological space can be summarized as follows.

- The topological order makes it possible to interpret and apply the coordinate system: the straight line can be mapped to the topological space, the sequence of points is unchanged, and the coordinates of a point are clearly fixed even when the topological space (or a domain of it) is mapped to another topological space (or to its domain).
- The topological order makes it possible to interpret and take a limit, including differentiation and integration: completeness makes it possible for point sequences to have an accumulation point; the separability allows the uniqueness of a limit.

## **3. Conditions and limitations of using topological tools**

In general, the condition of using any tool is also a limitation of using the tool.

### *3.1 Order, as a necessary condition*

The prerequisite for using topological tools is that the atoms and/or molecules that form the examined body, and in general the “particles” that make up the internal structure of the material should be in a fixed “order” and remain so under (and after) an effect on the body. It is also the most restrictive condition for the use of topological tools: the behavior of a body in which there is no topological order,

or if a resting topological order does not remain under an effect on the body, cannot be examined with the tools of topology.

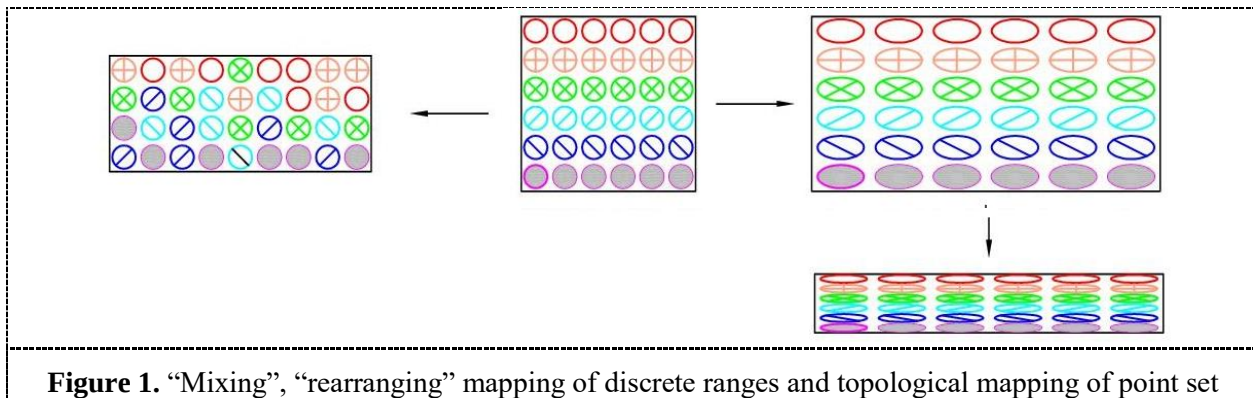
The basic idea of modeling: instead of the grid of atoms and/or molecules sitting in order in discrete points, we examine the points of a continuous point set, a domain of the Hausdorff space. The consequence of this is that the result obtained should not be referenced to any point of a domain of the Hausdorff space, but only to the reference point of each atom and/or molecule. In principle, this distinction is true, but it is irrelevant from a practical point of view: the human eye, the instruments used in everyday practice cannot distinguish an atom, but rather the location and position of a part of a material that can be well defined and incorporates a vast number of atoms and/or molecules; our examinations and measurements refer to such finite size “particles”.

The “transition” from the discrete point set to the domain of a topological space is made possible by the fact that “there is order” in the material at the atomic-molecular level. This is considered a basic assumption. Consequently, we can only examine such systems with the tools of the topology for which the basic assumption is met, and in this case the obtained results produce correct findings for the particles sitting on the points of the grid, or if there is no basic assumption of modeling, i.e. there is no topological order, then the interpretation of the obtained results should take into account that the underlying basic assumption is not correct. In the latter case, the atoms and/or molecules mixing with each other lose their unique marker, so in the description obtained with the topological means, the “result” may not refer to the particle to which the mapping is to be applied, but to another particle. This does not always mean that modeling is not able to describe the phenomenon examined within measurement accuracy. Think about the plastic forming of metals in which the degree of plastic rearrangement refers to a small part of the body. Such is the production of cold bent sections. In the plastic zone, we may not be able to precisely predict the location of all the metal atoms, but it can be predicted, for example, that a flat plate becomes an angled bend plate. However, in cases where “disorder” extends to the body as a whole, we cannot even estimate the location of atoms and/or molecules. Examples include kneading dough or Brown-movement of tiny, solid particles in liquids.

The requirement for a topological order sharply limits the application of modeling: even in the case of gaseous and liquid bodies, there is no order at all. In these cases, we cannot consider the material itself to be a domain of the Hausdorff space, because the constant movement of atoms and/or molecules makes it impossible to create an unambiguous correspondence between the “resting” gaseous and liquid body particles and the points of the Hausdorff space. Instead, we use a different “approach”: the embedding space is considered to be Hausdorff space, and we examine the mechanical characteristics of a particle of a matter flowing in space when it reaches the given point in space. That is, the topological order in the embedding space allows a continuous description of the flow. The flow of the body (granulated matter = powder, liquid, gas, the latter also requires thermodynamic formalism) is described in the embedded space as the topological space. The examined point is a fixed point of the embedding space, its place does not change; at this point in time different material particles pass through. We emphasize that we do not consider the material as a continuum, but consider the flow to be continuous, the flow itself occurs “*before*” a point set considered a continuum, as a coordinate system. That is to say that, the description model does not specify how a particle of a matter changes its location and velocity, and in fact does not specify the velocity of the particle arriving at a selected point in the space, but instead it determines the velocity of the particles arriving at a selected point in the space or in its small neighborhood will be roughly the same as that calculated in the model; at the same time, minor or major deviations are possible. In principle, the model is not accurate either if we assume that the flow lines never intersect, and accordingly, this flow model does not give any indication of the flow occurring in the flow perpendicular to the flow lines (the transverse diffusion).

Topological tools are suitable for determining the continuous mapping of two topologically equivalent ranges. This means that a topological mapping of a cube on to a sphere can be made, and a topological mapping among a rod, a disc, and a cuboid can also be produced. We know that the atoms and/or molecules themselves do not significantly change their size during mechanical effects. So, if we require the volume of the cube and sphere, or the rod, the plate, and the cuboid to be the same, i.e., they

consist of the same number of atoms (and/or molecules), then the atoms (and/or molecules) cannot be transferred from a spherical form to cube form, or among rod, disk, and cuboid forms by the topological mapping preserving the atomic-molecular structure. The explanation is trivial: finite-size atoms (and/or molecules) have to be rearranged, while in terms of points with no extension, two line segments of different lengths, two plane figures with different areas, and two bodies with different volumes (measured in some metrics) with the same (continuum) cardinality, can be mapped topologically, i.e. continuously and unique way one onto another. This means that during the shaping of the spherical dough into a cube, flattening it to a pie or rolling it into a roll, the alteration or rearrangement of the atomic-molecular order cannot be described by topological means (see Fig. 1.).



**Figure 1.** “Mixing”, “rearranging” mapping of discrete ranges and topological mapping of point set

The two examples above show that the use of topological devices within the body must have a topological order that must be maintained during (and after the cessation of) the effect; atoms and/or molecules cannot exchange place, disappear from the body to “nothing”, and cannot “join” to the body from “nothing”. This means that the reversible, elastic change of the shape of the solid bodies is a phenomenon that can be described without limitation by the topological description.

### 3.2 Strain and rearrangement

The body changes its shape under effect. The change of shape, from a topological point of view, can only be of two types: the topological order is preserved or the topological order does not remain. In order to distinguish between the two phenomena, in the first case we refer to strain and in the second case to rearrangement. Accordingly, during the flow of liquid, the atoms and/or molecules that make up the liquid are rearranged, the particles of soil under the influence of the penetrating effect of a pile are rearranged around the pile, at the same time, steel is subjected to strain during tension, bending and twisting. In the plastic formation of the metals, atoms are rearranged in the plastic zone, and strain occurs in the elastic zone.

### 3.3 The scale of the order and its kinematic degree of freedom

The topological order is usually “imagined” on two scales. One is the atomic-molecular order, and the other is a much larger order of magnitude, the built order; for example, a spatial frame structure or a system of uniform particles periodically contained in a matrix. In the first case, it is natural to identify the particle with the atoms, which in atom  $\rightarrow$  point modeling, we keep only three from the six degrees of kinematic freedom which three ones describe the displacement of the atom as a rigid body. In the second case, identifying the particle with a node of the frame structure, we feel that it is natural for a node in the frame  $\rightarrow$  point modeling to keep all six kinematic degrees of freedom of a node of the frame as a rigid body, i.e., three displacements and three rotations. Also, note that the stubs of the node stretch and shorten (imagining three rods, intersecting at one point as a node, these are three degrees of freedom), and that the angles of each branch of the node change (also three degrees of freedom at the same node). Most of the time, we also think of the particles embedded in the matrix similarly. In other words, when we switch to e.g. from a finite number of nodes in a frame structure to a continuum point

set as a mathematical model, then we want each point of the point set not to be three, but more, at least six, or possibly twelve kinematic degrees of freedom. This in itself is not special, think about the rigid body: the number of degree of kinematic freedom of it in the three-dimensional Euclidean space is six. At the same time, the space “including” of complete degrees of freedom, the “picked up” space for testing, is not physically the three-dimensional Euclidean space around us, but we constructed a space mathematically to perform the test. In the case of a rigid body, this is the six-dimensional phase space. The question is how many kinematic degrees of freedom are there for one (and so every) point in the set of points: equal to or more than the number of dimensions of the point set or possibly even more. A point in the point set has no size or an internal structure. Accordingly, neither rotation nor strain can be interpreted in relation to a point. Therefore, each point of a point set has exactly three degrees of kinematic freedom: three components of the displacement vector (assuming a three-dimensional space). Thus, the degree of kinematic freedom of the point set describes the displacement of the point set according to points, i.e. continuous mapping of a continuous manifold. Any other non-kinematic degrees of freedom other than displacement can be described by a function interpreted on the point set: e.g. body temperature, its electromagnetic state. To interpret the degrees of physical freedom, we do not increase the number of dimensions of space, nor do we consider the space as six-dimensional to describe the rotation of the rigid body in the three-dimensional Euclidean space.

The examined matter can be divided into matter containing structured parts (matrix) and particles; this way, the matter can be split into two parts.

Assuming that the topological order remains in both parts, there is the possibility of interpreting an embedded or generalized continuum. Take the case when the particles in the matrix are small. At this point, the location of the lifted parts of the matrix should be “removed”, and instead of a matrix we can consider a continuum. “Above” this is the system of lifted, periodically arranged particles. These particles are modelled with no-extension points. Only displacement will remain as the degree of kinematic freedom. Because there is a finite amount of them, the topology of the point set can be interpreted, but in this case a limit can not be taken. Additionally, to merge the two systems, the points must be “replanted” in the topological space modelling the matrix. However, there is no place there for another point; because we consider the topological space to be complete (otherwise it would not be possible to take a limit in a unique way). Consider the case when the particles in the matrix are large. At this point, the location of the lifted particles in the matrix can not be “eliminated”, and the matrix should be seen as a multiple connected continuum leaving the place of particles empty. “Above” this is the system of lifted, periodically arranged particles. These particles can be modelled as a rigid or deformable solid body. In this case, the degree of freedom is not only the displacement, but also the rotation and the internal deformation. In this case, a limit can be interpreted within a particle (the particles themselves can also be considered as a domain of a topological space), but because of the finite amount of them, the sequence passing through from one particle to the other cannot be interpreted and so there cannot be interpreted a limit in the case of particle set. (The topology of particle set can be interpreted in principle, see [13,14], but between disjunct domains, differential and integral calculations cannot). Furthermore, to unite the two systems, it is necessary to “replant” the particles in the topological space modeling the matrix. It is true that we left its place out, but we need to establish a connection between the lifted and replanted particles and the matrix that accommodates it (if you like, the neighborhoods that run on the two “boundary” surfaces must be merged into one), then the movement of particles independent of the matrix (revitalized by embedding) prevents it. (So, the lifted particles and the hole left in the matrix may be deformed differently, so the particles, which are deformed independently of the matrix, cannot be replanted into the matrix that deformed differently from particles. The condition of replantation is exactly this; an identical deformation of the mutual surfaces. In other words, they are non-autonomous continuums: the displacement vectors for the right and left sides of the contact surface are the same. This system can be considered as a continuum the material characteristics of which change with jump along one (or more) internal surfaces. This does not make the matrix and the granules separate into two individual continuums, or the two jointly into a generalized continuum.

### 3.4. Overview of topological characteristics of modeling matter

The following elements of the topological characteristics are highlighted. The number of “particles” that make up the model; its number can be finite or a continuum. Is there a topological order among the particles forming the model before deformation? Is there a topological order between the particles forming the model during deformation? Is the mapping of “particles” - their relative movements - continuous or discrete during deformation? Based on these topological features, the models can be divided into the following main classes.

*Classical continuum.* Continuum number of a set of points. There is a topological order before the deformation (mapping). The mapping is continuous. The topological order between the points remains during and after the mapping. The point making up the continuum, i.e. “particle” has no size, no internal structure. The degree of kinematic freedom is displacement. The functions used to describe the system are interpreted over the continuum as an interpretation domain [1,2]. Within the classical continuum as a model, the use of fracture conditions allows for the description of larger scale discontinuities, such as the determination of the surface of the plastic behavior area or of fracture surfaces in granular media. Within the classical continuum as a model, it is possible to describe rapid or stochastic variables by using averaging and homogenization methods [15,16,17,18].

*Grid continuum (generalized continuum).* Finite number of the set of points. There is a topological order before deformation. The mapping may also include continuous (collective, acoustic) and discrete (individual, optical) motion forms. The topological order between the points remains during and after mapping [19]. The point making up the grid continuum, that is, the “particle” has dimensions, has an internal structure. The degree of kinematic freedom may be rotation, elongation, angular variation, the second-order deformation tensor commonly used in the classical continuum, or the richer (multi-parameter) form that describes the shape change. Three (main) representations can be distinguished. One is to represent the “particles” in the grid point with directors. Then the relative change in the length of the directors and the change of angle between the directors give the degrees of kinematic freedom. The second is to classify the “particles” in discrete grid points into cells, and to group the individual degrees of freedom of displacement of the points in the cells into different types of strain, such as tension, shear, bend, or strain that are common in classical continuum mechanics. The third is that besides the functions describing the system, their gradients are also treated as unknown quantities. To describe the system, the grid continuum is embedded into an external space considered as the domain of functions describing the system, but not the entire set of values but only the values over grid points are applied to describe the grid continuum [20,4,5,19,21,22,23].

*Granular medium.* Finite number of the set of points. There is a topological order before deformation. The mapping can be continuous (the stress set of particles are in equilibrium due to the effects of external forces) and may be non-continuous (some parts of the particle set or the whole is rearranged for equilibrium). The particle forming the medium has dimensions and an internal structure. The degree of kinematic freedom is the displacement and the rotation, and in some cases the strain degree of freedom can be assigned to it. The functions used to describe the system are interpreted above the space enclosing the particles as the domain of interpretation. For a small number of particles, state equations for each particle are written. In the case of a large number of particles, the set of particles is modeled as a medium, and the functions for each particle areas considered continuous functions in the embedding space over the domain of interpretation. Usually both the classical and the generalized continuum models are used. In these cases, the state functions are applied to a larger volume of particles (if the value is “averaged”) [24,25,26].

*Liquids and gases.* The set of particles consists of a finite number of “particles”. There is no topological order in liquids or gases. Statistical methods can be used primarily to describe the state. The continuous description should exclude that the particles are “disordered” relative to one another: this “chaotic” state is “smoothed”, and it is considered that the particles forming the liquid and or the gas have a topological order relative to one another. With this condition, the mathematical apparatus offered by both the classical continuum and the grid continuum becomes applicable. At the same time, when interpreting the results obtained, one has to consider the fact that the solution was obtained by smoothing

the chaotic behavior, in reality there is chaotic movement, and even some flows would not be created without chaotic behavior.

#### 4. Summary

In this paper, we have reviewed the possibilities and limitations of using topological tools.

Continuous mapping, differential and integral computation are referred to as topological tools.

The conditions for using topological tools are as follows:

- the particles that form the material to be modeled, let the particles be atoms and/or molecules, or larger-scale elements such as particles or cells of a constructed structure, must have a topological order,
- the material to be modeled must be replaced by either a topological space or the points representing one cell must be embedded in a topological space.

The consequences of using topological tools are as follows.

- Three types of models can be obtained
  - o material flowing before the continuum (particle, liquid or gas),
  - o classical continuum,
  - o grid continuum or generalized continuum.
- By modeling the material flowing before the continuum, information about either the rearrangement of the flowing material or from the transverse flow perpendicular to the flow lines cannot be obtained.
- Classical continuum (continuum number of the set of points)
  - o freezes internal degrees of kinematic freedom: only (continuous) displacement can be interpreted, independent rotational degree of freedom cannot,
  - o the internal kinematic degrees of freedom can only be continuous: the displacement of two adjacent points is almost identical, only points between which there are several additional points can move face to face.
- The grid continuum or generalized continuum (finite number of the set of points, embedded into a point set of continuum cardinality)
  - o preserves the degree of internal kinematic freedom: besides the displacement, the independent rotation can be interpreted, as well as any other degree of kinematic freedom in connection with the change of the shape of the solid body sitting in the node points of the grid continuum, or the cells form by the solid bodies sitting in the node points of the grid continuum,
  - o the internal degree of kinematic freedom can be both continuous and discrete: the displacement, rotation, change of shape of two adjacent “points” can be almost the same, i.e. continuous, but two neighboring “points” can shift and rotate face to face, their strain states may be opposite,
  - o continuous state functions only have mechanical content applicable to elements of the grid points in the node points of the grid continuum.

Findings analogous to kinematic degrees of freedom can also be made for dynamical degrees of freedom (stresses, internal forces).

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