Exploratory analysis regarding the domain definitions for computer based analytical models

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Abstract. Our previous computer based studies dedicated to structural problems using analytical methods defined the composite cross section of a beam as a result of Boolean operations with so-called ‘simple’ shapes. Using generalisations, in the class of the ‘simple’ shapes were included areas bounded by curves approximated using spline functions and areas approximated as polygons. However, particular definitions lead to particular solutions. In order to ascend above the actual limitations, we conceived a general definition of the cross sections that are considered now calculus domains consisting of several subdomains. The according set of input data use complex parameterizations. This new vision allows us to naturally assign a general number of attributes to the subdomains. In this way there may be modelled new phenomena that use map-wise information, such as the metal alloys equilibrium diagrams. The hierarchy of the input data text files that use the comma-separated-value format and their structure are also presented and discussed in the paper. This new approach allows us to reuse the concepts and part of the data processing software instruments already developed. The according software to be subsequently developed will be modularised and generalised in order to be used in the upcoming projects that require rapid development of computer based models.

1. Introduction
Computer based approaches use analytical components in all the types of models, for instance in numerical models, in experimental data processing and, certainly in analytic models. Most of the models may be expressed in terms of functions. For instance, analytical models based on the strength of materials theory are using:
• functions depending on the geometry and on the dimensions of the cross section to calculate the geometrical characteristics;
• functions depending on the loads and supports to calculate the internal forces and moments;
• functions depending on the geometry, on the geometrical characteristics and on the internal forces and moments to compute the stresses;
• functions depending on the geometry, on the geometrical characteristics and on the internal forces and moments to compute the deflections.
In all these cases the geometry appears either as an explicit condition, or as an implicit one. It results that the geometry of a model and its dimensions are variables of the previously mentioned functions, therefore the geometry related problems require a thorough analysis. Moreover, the geometry is actually a domain from which the according function is extracting its input variables.
2. Theoretical background

New engineering problems require creative approaches and sometimes new computing instruments. A basic question we should ask when a new solution is necessary regards the possibility to create a computer aided instrument that may be used to solve all that given class of problems. Conceiving computer based solutions is helpful from several points of view:

- it requires a thorough analysis of the problem and of its context, in this way leading to a better understanding of that field of science;
- it solves an entire class of problems if a flexible computer based solution is conceived;
- it allows connections with other problems for which we already developed computer based instruments, i.e. knowledge integration, [1].

Automatic calculus of the structural problems using strength of materials and theory of elasticity analytical methods is a long run concern of the authors, [2] [3] [4]. In this way, in [2] we present a computer based analytical method used to compute the geometrical characteristics of the cross sections and of the stresses. The cross section is composite, being the result of some Boolean operations with rectangles and circles, i.e. ‘simple’ shapes. Once the principle of the calculus method was being proved, the concept was generalised by including in the set of the ‘simple’ shapes other shapes for which we may use either direct calculus relations, or calculus algorithms.

The first generalisation level was based on the approximation theory, a curve being approximated by a set of spline functions, [5]. In this case, the curve is a boundary of the ‘simple’ shape, its frontiers being approximated by spline functions. We conceived a general method to compute the geometrical characteristics for such sections bounded by spline functions, [3].

The second generalisation level was based on the approximation of an area by a set of polygons, [4]. In this case we also have direct calculus relations of the geometrical characteristics. The accuracy of this method was tested for mechanical parts with rounded fillets, in order to identify the number of points which best fit the circular arc. Finally, any area may be divided in a set of triangles, i.e. a curved boundary can be approximated by a line segment.

Third direction of generalisation may be suggested by starting from the same cross section related approach. Let us consider that we have an inhomogeneous section, made of several materials. In this case the area of each material may be approximated using one of the previously mentioned methods. However, each area has particular material constants that must be accordingly assigned.

To conclude, the cross section related approach was generalised from several points of views. Notwithstanding these strengths consisting of the generalisation methods that were tested, there are some weak points that must be identified and according solutions must be conceived.

3. Discussion

The previous generalisation methods were tested in the particular context of the cross sections related approach. This means that the calculus of the geometrical characteristics was an important goal of the study. However, along the section the variation of the first moment of area is important in Juravski’s relation used to compute the shear stresses. Moreover, for the calculus of the form factors for shear, other function must be integrated.

Another weak point is related to the customised definition of the material constants assigned to each area of distinct material of the section, in this way being defined particular cross sections.

Last but not least, all the examples presented in the aforementioned papers were given for simple and relevant cross sections having particular shapes.

3.1. Main ideas to ascend from particular sections to the general definition of the calculus domains

Let us consider a meta-level from which the previous problems and solutions may be reassessed. Despite the previous particular definitions of the sections, general solutions were conceived. However, the degree of generality of a solution is limited by the particular definition of the problem. To overcome this aspect, we consider that a cross section may be regarded as a calculus domain consisting of several subdomains. The definitions of the subdomains are in accord with the algorithms
presented in [3] and [4], i.e. as subdomains whose boundaries are curves approximated either by spline functions, or by line segments. Moreover, the material constants of the previous particular problem may be regarded as metadata assigned to each subdomain.

The new general vision must be analysed from several points of view, in order to answer the following questions:
- The new approach allows reusing of previously developed concepts, software instruments and practical applications?
- What is the most flexible method to define the domains in order to offer an upper level of generality and usefulness to this new approach?
- What new problems may be solved using this new vision?

3.2. Reusability of the prior work
The new approach does not completely changes the problems already solved, i.e. the computer based solutions. However, the domains previously defined as particular sections must be redefined using the actual general grounds. The applications that use general datatypes may be reused to solve the new redefined problems.

3.3. Domain definition
The usefulness of the calculus method is given by the flexibility of the algorithms and in particular, by the computer wise definition of the input data.

First of all, the input data must be easily defined using some of the most common resources of an operating system. As we successfully used in our software projects text files where the input data was expressed in comma-separated-value (CSV) format, this type of input data will be also used in this project.

Figure 1. Structure of the text file where a domain is defined.

Figure 2. Types of definitions of a subdomain.

Figure 1 presents the main information used to define a domain, i.e. the number of subdomains, and for each subdomain: the identifying index, the sign, the type and a string which represents the name of the CSV file where the current subdomain is defined. Sign is used for Boolean operations with the subdomains and it is +1 for a ‘solid’ subdomain that is added to the domain, or -1 for a ‘hollow’ subdomain that is subtracted from the domain.

Figure 2 presents the two methods used to define a subdomain, i.e. either by its set of boundaries (spline functions or line segments), or as a polygon (area of the polygon is the area of the subdomain).

Figure 3 presents the structure of the information that is necessary to define a subdomain using its boundaries, the according CSV file consisting of lines which represent the filenames of the text CSV files where the following information is stored: definition of the line segments, definition of the spline functions, definition of the inner point and metadata assigned to the current subdomain.

The text CSV file that defines the current line segment consists of two lines that represent the filenames of the CSV files where the list of points is stored (identifying index and coordinates) and the list of connections (flag regarding the current segment and the identifiers of the vertices of the segment). The flag of the current segment is 1 if the segment is on the boundary of the domain, or 0 if it is an inner side, i.e. it defines two polygons of the domain.
The CSV file that defines the spline functions stores:

- the identifying index of the current spline function, \( i \);
- the horizontal coordinate of the left end of the current interval, \( x_i \);
- the horizontal coordinate of the right end of the current interval, \( x_{i+1} \);
- the coefficients of the current spline function, i.e. \( A_i \), \( B_i \), \( C_i \) and \( D_i \).

The curve approximated by spline functions may be defined as:

\[
y(x) = \sum_{i=0}^{N} \left( H(x-x_i) - H(x-x_{i+1}) \right) \left[ A_i \cdot (x-x_i)^3 + B_i \cdot (x-x_i)^2 + C_i \cdot (x-x_i) + D_i \right],
\]

where \( H(x) \) is Heaviside’s step function.

| Subdomain defined by the boundaries - csv file |
|-----------------------------------------------|
| Line segment definition - csv filename         |
| Coordinates - csv filename: point index, x, y, z |
| Connections - csv filename: segment type, node1, node 2 |
| Spline functions definitions - csv filename   |
| Inner point coordinates - csv filename: point index, x, y, z |
| Attributes of the subdomain - csv filename: explanation, symbol, unit, value |

\textbf{Figure 3.} Structure of the information used to define a subdomain using its boundaries.

The so-called ‘inner point’ is used to define the inner region of the subdomain. For instance, the point of reference has the coordinates \((x_R, y_R)\) and the point to be tested if it is included in the subdomain has the coordinates \((x_T, y_T)\). If this point is included in the domain, it is fulfilled the condition \( f(x_R, y_R) \cdot f(x_T, y_T) \geq 0 \), where \( x_i < x_T < x_{i+1} \). For line segments that define a polygonal area there may be used specific conditions to test if a point is included in that area.

Attributes of the subdomain are meta-information regarding the subdomain and they are stored in a distinct text CSV file. In this way, an indefinite number of parameters may be assigned to the current subdomain. For a cross section, this file may store the information regarding the current subdomain, such as: designation of the material, the Young’s modulus, Poisson’s ratio, allowable stress and others.

Figure 4 presents the necessary information to define a subdomain as a polygon. The CSV text file that defines the subdomain stores the designation of the CSV text file that defines the polygon and the designation of the file that defines the attributes. Similar to the file that defines the line segment, the file that defines the polygon includes the designation of the file where the vertices related information are stored and the designation of the text file where the connections are defined. For the polygons we have the direct calculus relations presented in [3], where are also presented advices regarding the enhancement of the accuracy for fillets’ arcs that must be discretized using an angle smaller then \( 10^\circ \).

The text CSV file, figure 4, where the meta-information are stored is similar with the one presented in figure 3, being stored the same types of attributes.
If in an application there must be defined several domains, i.e. several cross sections of a three-dimensional definition of a structural problem, the information regarding the domains is stored in the configuration file of the application, figure 5. The first line is the number of domains, followed by pairs of two lines. The first line is the path where the domain definition file may be found, in this way being suggested to store the information specific to a domain in a distinct folder. The designation of the domain related CSV file is stored in the following line of the file whose structure is presented in figure 1.

![Configuration csv file](image)

**Figure 4.** Structure of the information used to define a subdomain as a polygon.

**Figure 5.** Structure of the configuration file that may consider the definition of several domains.

The configuration file previously presented is the first file that is opened and read by the current application, so it is in the topmost position of the hierarchy of files.

![Sample information stored in a configuration file viewed using NotePad++ and Excel](image)

**Figure 6.** Sample information stored in a configuration file viewed using NotePad++ and Excel.

To have an explicit method of structuring the information that may be verified in running conditions by tracing the execution, it is useful to store in the first column the meaning of the information stored in the second column; in the second column is stored a string datatype whose significance is the path or the CSV filename. In this way, the application identifies the functionality of
the information stored in the second, the third and all the other columns. This method may be very useful in the CSV file that stores the meta-information assigned to each subdomain.

3.4. New types of problems that may be modelled
The new vision regarding the domain general definition allows us to approach new types of problems. A wide range of problems where metadata are assigned to the subdomains are the metal alloys equilibrium diagrams or the multicomponent phase diagrams.

![Figure 7. The Fe-C equilibrium diagram, [6].](image)

This type of problems uses attributes assigned to each subdomain, i.e. phase of the diagram. An interesting study regarding the solidification of a steel is presented in [6], paper that provides the coordinates of the points presented in figure 7. These points, together with some other points picked up by us in order to best fit the curves, may be used to define the diagram as a Boolean summation of subdomains.

Other problem where metadata may be stored for parts of a region is in the map-wise representation of the information, including for maps.

Last but not least, it is interesting how this domain definition approach may be used for more complex shape-related problems, such as the pattern or shape recognition, [7]

4. Conclusions
General definition of the calculus domains was a logical step that should be followed for developing flexible and reliable computer based instruments.

Despite the general solutions previously developed by us, a profound parameterized definition of the domains will provide wider knowledge horizons, to be used in the accurate modelling of new phenomena in several fields of science, not only in engineering.

We continue to study the best methods to conceive flexible and general definitions of the subdomains, which may be regarded as Lego pieces used to create accurate representations of the real domains.

Using modularization and reusability of the according software, we will design the necessary libraries of flexible programs for the rapid development of various computer based models.

All these components provide new methods to define calculus domains, i.e. new intelligent means to investigate phenomena and to acquire knowledge using computer aided modelling, that lead to a metalevel of understanding.

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