TUTORIAL SURVEY

POROUS FUNCTIONS – II

Iryna Trymorus, Igor Podlubny

Abstract

A new mathematical tool, porous functions, has been suggested recently. In this paper operations with porous functions are further discussed alongside with computational tools, which are necessary for evaluation of porous functions, their visualization, and basic operations with such functions in two- and three-dimensional cases.

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1. Introduction

Recently a new approach to modeling the structure of real materials have been introduced [1], based on a new kind of functions – *porous functions*, with possible applications to modeling various types of real-world materials (granular, porous, composite, etc.) and structures (city agglomerations, forests, etc.) and dynamical processes in such materials and structures. This approach was presented at several conferences [2, 3, 4] in order to verify its viability and potential applications.

In this paper, we further and in more details explain the notions related to porous functions and basic operations with them, including visualizations, computations, and example of code for using the Porous Functions Toolbox (PFT) for MATLAB [2, 5, 6].

2. Cells, Grains, and Pores

As it was introduced in [1], a porous interval is divided into *subintervals*. A *subinterval*, consisting of a bounding box (a minimal rectangular container (in three-dimensional case, it is a parallelepiped) which tightly encloses a grain/pore, is denoted as a *cell*. The same term is used for the abstract class *cell* used in PFT for representing grains and pores in two- and three-dimensional cases.

```
classdef (Abstract) cell
    properties
        shifts shifts2d %shifts3d
        cellData cellDataInterface
        boundingBox bbBox
    end
end
```

The *shifts2d* (*shifts3d* for 3d case) property contains a relative position of a cell inside a porous interval. The width (δx [1]) and shape of a grain/pore is defined by the *cellData* property of a class type inherited from *cellDataInterface*. This allows the creation of any type of cell: of selected standard shapes (circle/sphere, rectangle/parallelepiped, square/cube) or custom shape (irregular, or user-defined shape).

Since *cellDataInterface* requires only coordinate points of a grain/pore, all details of generating are hidden into derived classes. Thus, PFT contains two separate classes: *grain* (for creating filled cells – an analogy of some physical material of self-similar structure, such as sand) and *pore* (for creating void cell to represent foam-like materials). For instance, an ellipse-shaped grain (Fig. 2.1) or pore (Fig. 2.2) can be formed by using *ellipseCellData* (*ellipsoidCellData* for 3d case).

FIG. 2.1: Grains and their cells

FIG. 2.2: Pores and their cells

Let us illustrate how to create cells shown on Fig. 2.1 and Fig. 2.2 using PFT.

```
%% build grain for 2d case
% set prerequisites
cellData = ellipseCellData(1, 1);
shifts = shifts2d(5, 10);
% create grain
grain2d = grain2d(cellData, @bbox2d, shifts);
%% build grain for 3d case
% set prerequisites
cellData = ellipsoidCellData(1, 1, 1);
shifts = shifts3d(5, 10, 15);
% create grain
grain3d = grain3d(cellData, @bbox3d, shifts);

%% build pore for 2d case
% set prerequisites
cellData = ellipseCellData(1, 1);
shifts = shifts2d(35, 10);
% create pore
pore = pore2d(cellData, @bbox2d, shifts);
%% build pore for 3d case
% set prerequisites
cellData = ellipsoidCellData(1, 1, 1);
shifts = shifts3d(35, 10, 15);
% create pore
pore = pore3d(cellData, @bbox3d, shifts);
```

Grains/pores are essential components of porous intervals, as they provide the characteristics used in describing the properties and behavior of the structure as a whole.

3. Porous Intervals

3.1. Notation. A porous interval is denoted as [1]

$$I_p = \{[a, b], \delta x, \mu(x)\}, \quad (3.1)$$

where a and b are the lower and the upper bounds (we can think of them as lines in the two-dimensional case, or planes in the three-dimensional case),

δx is the grain/pore width, and $\mu(x)$ is the rule describing the distribution of grains/pores (either stochastic or deterministic).

Let also denote a grain/pore height as δy and consider $\mu(x)$ as $\mu(x; h, \delta y)$, where $h = |b - a|$ is the height of I_p . This $\mu(x; h, \delta y)$ generates a set of K integer numbers, which we denoted J (*indices* of cells in I_p), where

$$J = \{k : k \in E(\mu(x; h, \delta y))\}, \quad (3.2)$$

where E is the range of the function $\mu(x; h, \delta y)$, representing the distribution rule based on h and K , $K = \lfloor h/\delta y \rfloor$ is the number of cells that fit in I_p . Thus, a porous interval can be described as an indexed family of cells with an indexed set J

$$I_p = \{C_j\}_{j \in J}, \quad (3.3)$$

where C_j is a set of cells, containing only one cell (3.4).

$$|C_j| = 1. \quad (3.4)$$

3.2. Creating porous intervals in PFT. An algorithm for creating and handling a porous interval object I_p in PFT is based on the cells described in Section 2, and custom classes and interfaces for I_p are provided in the PFT. The class *pi2d* (and *pi3d* for the three-dimensional case) is the basic one, which allows the creation of I_p and manipulations with it: visualization (draw), refill (regenerate indices of cells), performing of basic operations. It is characterized by the following properties:

```

classdef pi
    properties (Access = protected)
        cellsFactory cells2dFactory (cells2dFactory)
        container intervalContainer
        indices (1, :) double {mustBePositive, mustBeFinite} = 1
        cells (1, :)
    end
end

```

The *cellsFactory* property is a factory that generates a cell of defined shape and size. It also contains methods for calculating the size characteristics of a porous interval.

The *container* property represents the constraints of I_p based on the cell sizes ($\delta x, \delta y$ and eventually δz in the three-dimensional case) and the interval height h . It has a rectangular shape (or parallelepiped in the three-dimensional case), but can be customized as necessary.

The *indices* property represents an array with the indices of the cells positions, distributed following the distribution rule $\mu(x; h, \delta y)$. This class also provides necessary auxiliary internal properties and methods, which we do not need to list here.

The basic algorithm for creating a porous interval I_p is the following:

- define the cell type (shape, size),

- define the interval $[a, b]$ to build a container for the porous interval,
- define a distribution rule/law $\mu(x; h, \delta y)$, and generate unique indices of cells of the porous interval,
- place the cells to corresponding calculated positions.

This algorithm is implemented in the method *fillInterval* of *pi* class and as a result initiates the *cells* property.

How it works can be illustrated by running the following code snippet, which generates I_{p2d} and I_{p3d} (Fig. 3.1), filled by the grains described in Section 2 (i.e. elliptical grain with dimensions equal to 1):

```
%% build pi2d
% set cell type
cellData = ellipseCellData(1, 1);
% define pi position
shifts = shifts2d(5, 15);
% define pi height
height = 30;
% define pi container type
container = parallelepipedIntervalContainer(cellData, shifts, height);
% define distribution law scale
scale = 0.4;
% define distribution law type    uniform
dr = uniformDR(scale);
% generate indices
indices = dr.generateIndices();
% initialize cells factory
cellsFactory = cells2dFactory(cellData, @bbox2d);
% create pi
pi_1 = pi2d(cellsFactory, container, indices);

%% build pi3d
% set cell type
cellData = ellipsoidCellData(1, 1, 1);
% define pi position
shifts = shifts3d(5, 10, 15);
% define pi height
height = 30;
% define pi container type
container = parallelepipedIntervalContainer(cellData, shifts, height);
% define distribution law scale
scale = 0.4;
% define distribution law type    uniform
dr = uniformDR(scale);
% generate indices
indices = dr.generateIndices();
% initialize cells factory
cellsFactory = cells3dFactory(cellData, @bbox3d);
% create pi
pi_1 = pi3d(cellsFactory, container, indices);
```

FIG. 3.1: Examples of I_p

4. Distribution of Grains and Pores

The distribution rule/law $\mu(x; h, \delta y)$ plays a significant role for porous intervals and porous functions, as it is used to assign a cell (grain, pore) to a particular place. The PFT toolbox provides the *drInterface* class, which allows to use any mathematical algorithm for generating cell indices (random using any CDF – cumulative distribution function, or any deterministic distribution rule). Several classical CDFs (uniform distribution, normal distribution, etc.) are already implemented and can be used immediately.

```
% Indices distribution rule
classdef drInterface < handle
    properties
        % percentage of interval's which will be filled by cells
        scale
        % interval = [start_val end_val]
        interval
    end
    methods (Abstract)
        % returns an array of indices inside interval distributed
        % accordingly to some algorithm
        generateIndices(obj);
    end
end
```

The distribution rule $\mu(x; h, \delta y)$ uses the scale value $\rho \in [0, 1]$ (the density of the distribution rule), that defines the percentage of I_p filled by cells. The value of $\rho = 1$ means that the porous interval is completely filled by cells (grains/pores).

5. Porous Functions

5.1. **Notation.** A porous function F_p is described as

$$F_p = \{I_p, \begin{bmatrix} v(x) \\ u(x) \end{bmatrix}, \phi, \mu(x; h, \delta y)\}, \quad (5.1)$$

where ϕ is a function describing the cell type (a grain/pore shape and size).

In addition to the lower shape $u(x)$ [1], let us denote by η the constraints of a physical container. The function $u(x)$ can be considered as one of the constraints, that $u(x) \in \eta$.

Using the setx notation, F_p can be denoted as an indexed family of porous intervals I_p (3.3)

$$F_p = \{I_{p_i}\}_{i \in I}. \quad (5.2)$$

For a porous function of one variable we have:

$$I = \{k : k \in D(v(x)); k_m = k_{m-1} + \delta x\}, \quad (5.3)$$

where $D(v(x))$ is the domain of a shape function $v(x)$.

For a porous function of two variables:

$$I = \{(k, d) : k, d \in D(v(x, y)); k_m = k_{m-1} + \delta x; d_n = d_{n-1} + \delta y\}, \quad (5.4)$$

where $D(v(x, y))$ is the domain of a shape function $v(x, y)$.

In the case of a porous interval I_p , where every element of an indexed set J links to a set of only one cell (3.4). However, the set of indices I in (5.3) and (5.4) links to a set of porous intervals, which are located on the same spatial coordinates – the situation that occurs during shape or body addition of porous functions.

5.2. **Creating porous functions in PFT.** For creating or evaluating a porous function F_p the following algorithm is used:

- define upper shape functions $v(x)$ [1] ($v(x, y)$ for 3d case);
- define a distribution rule $\mu(x; h, \delta y)$ ($\mu(x, y; h, \delta z)$ for 3d case);
- define constraints η ;
- define the cell shape and size ($\delta x, \delta y$ (δz for 3d case) [1]);
- calculate the values of $v(x)$ ($v(x, y)$ for 3d case) for each value of x (x, y for 3d case).
- for each value of the shape function build the corresponding porous interval I_p as described in Section 3.2.

In the PFT toolbox, this algorithm is implemented as a set of custom classes for handling porous intervals described earlier, and the *pf2d* class (*pf3d* in the three-dimensional case), that includes the main properties and methods to initialize, build, draw and handle operations with porous functions:

```

classdef pf
    properties
        shapeFunction shape2dFunction % shape3dFunction for a shape
                                function of two variables
        pisFactory pi2dFactory % pi3dFactory for 3d case
        container container2dInterface % container3dInterface for 3d case
        intervals keyArrayMap % key pair collection of porous intervals
    end
end

```

The *shapeFunction* property represents the shape function $v(x)$ of a porous function F_p . It can be of one variable or of two variables (implemented in *shape2dFunction* and *shape3dFunction* classes, respectively).

The purpose of the *pisFactory* property is similar to *cellsFactory* – it generates I_p based on *shapeFunction* value for specific x (or x and y in three-dimensional case), a distribution rule $\mu(x; h, \delta y)$, and a cell type.

The *container* property plays the role of a 'physical container', that holds some porous material, described by F_p .

For creating a custom container, a new container class derived from *container2dInterface* (or, *container3dInterface* in the three-dimensional case) must be defined. In this way, any necessary type of an external F_p container can be created.

The *intervals* property represents a custom data collection of I_p of a type *keyArrayMap*, that is based on the built-in MATLAB type *containers.Map*, but with a possibility to use a numbered pair as a key to index every I_p by its location coordinates (x in the two-dimensional case, $[x, y]$ in the three-dimensional case).

The porous function, generated by the following code snippet, is shown in Fig. 5.1:

```

%% pf3d
% set cell type
cellData = ellipsoidCellData(1, 1, 1);
cellsFactory = cells3dFactory(cellData, @bbox3d);
% set porous intervals factory
scale = 0.5;
dr = uniformDR(scale);
pisFactory = pi3dFactory(dr, cellsFactory,
    @parallelepipedIntervalContainer);
% set shape function
shapeFunc = shape3dFunction('x + y');
% define external (physical) container with the following characteristics
% parallelepiped with 2 <= x <= 10; 3 <= y <= 20; 10 <= z <= 40;
boundaries = boundaryIntervals3d(
    boundaryInterval(2, 10),
    boundaryInterval(3, 20),
    boundaryInterval(10, 40));
pfContainer = parallelepipedPFContainer(boundaries);
% build porous function
pf = pf3d(shapeFunc, pisFactory, pfContainer);

```

 FIG. 5.1: Examples of F_p

As one can see in Fig. 5.1, a physical container can extend the maximum value of the shape function ($\max(v(x_0)) < \eta(x_0)$), which means that there will be left some free space (not filled by cells). It can be filled later by another type of porous material (like in body addition). In the case when a physical container is smaller than the value of the shape function ($v(x_0) > \eta(x_0)$), the porous function is cropped to the level of the container border ($v(x_0) = \eta(x_0)$).

It can occur that there will be some space not filled by grains or by pores; this happens due to the approximation of the shape function by a rectangular (or parallelepiped in three-dimensional case) porous intervals and the fact that a porous interval cannot always be completely filled by cells because the height of the porous interval can be divided by the height of a cell with a remainder.

6. Equality of porous functions

DEFINITION 6.1. Consider two porous functions F_p^1 and F_p^2 :

$$F_p^1 = \{I_p^1, \begin{bmatrix} v^1(x) \\ u^1(x) \end{bmatrix}, \psi^1, \mu^1(x; h^1, \delta^1 y)\}, \quad (6.1)$$

$$F_p^2 = \{I_p^2, \begin{bmatrix} v^2(x) \\ u^2(x) \end{bmatrix}, \psi^2, \mu^2(x; h^2, \delta^2 y)\}. \quad (6.2)$$

Two porous functions F_p^1 and F_p^2 are *equal* ($F_p^1 = F_p^2$), if all their characteristics are equal:

$$I_p^1 = I_p^2, \begin{bmatrix} v^1(x) \\ u^1(x) \end{bmatrix} = \begin{bmatrix} v^2(x) \\ u^2(x) \end{bmatrix}, \psi^1 = \psi^2, \mu^1(x; h^1, \delta^1 y) = \mu^2(x; h^2, \delta^2 y). \quad (6.3)$$

FIG. 6.2: Absolutely equal porous functions

As a porous function can include randomization due to the use of a distribution law/rule, two porous functions can be *equal* in the sense of Def. 6.1, but their visual representations can differ. Thus, let us define the *absolute equality*, when in addition to the previous the equality of all cell locations is required.

DEFINITION 6.2. Two porous functions F_p^1 and F_p^2 are *absolutely equal* ($F_p^1 \equiv F_p^2$), if

$$F_p^1 = F_p^2, \quad I^1 = I^2, \quad (6.4)$$

where I^i ((5.2)) are compared in the terms of the equality of sets.

In Fig. 6.1 two equal porous functions are depicted. It is easily seen, cells have different values: grains and pores occupy different cells of the same porous intervals. In Fig. 6.2 two absolutely equal porous functions are shown: all grains and pores are at the same positions.

FIG. 6.1: Equal porous functions

Every time the *build* function of *pf* class is called after the creation of porous interval using some probabilistic distribution law, new cell indices are generated, hence equal (but not absolutely equal) porous functions are built.

7. Addition of Porous Functions

Two possible approaches to addition of porous functions were outlined in [1]: the shape addition and the body addition.

7.1. Shape addition. Consider two porous functions F_p^1 and F_p^2 :

$$F_p^1 = \{I_{p_i}^1\}_{i \in I^1}, \quad (7.1)$$

$$F_p^2 = \{I_{p_i}^2\}_{i \in I^2}, \quad (7.2)$$

DEFINITION 7.1. Shape addition $\cup^s$ is defined as

$$F_p^1 \cup^s F_p^2 = \{I_{p_i}^1 \cup^s I_{p_i}^2\}_{i \in I^1 \cup^s I^2}, \quad (7.3)$$

where

$$I_{p_i}^1 \cup^s I_{p_i}^2 = \{C_j\}_{j \in J^1} \cup^s \{C_j\}_{j \in J^2} = \{C_j\}_{j \in J^1 \cup J^2 + h}, \quad (7.4)$$

$$I^1 \cup^s I^2 = I^1 \cup I^2 \cap I_\eta, \quad (7.5)$$

and I_η is the set of all possible indices of porous intervals in the η container.

The shape addition of porous functions is based on the shape addition of its porous intervals in the corresponding positions. One porous function can be defined on the wider, bigger container, meaning that some (or even all) interval positions can differ.

If the first porous function is “wider”, it does not create any problem, because all porous intervals of the second porous function can be added. However, if the height of these intervals exceeds the external container, it will be cropped to the container boundaries. In the second porous function is “wider”, its intervals are cropped to the container boundaries in all directions.

The following code snippet illustrates how the shape addition of two porous functions F_p^1 and F_p^2 is performed with the help of the method *addShape* provided by the class *pf* of the PFT toolbox. The result is shown in Fig. 7.1.

```
%% shape addition of pf1 and pf2
% pf1
% set cell type
cellData = ellipsoidCellData(1, 1, 1);
cellsFactory = cells3dFactory(cellData, @bbox3d);
% set porous intervals factory
scale = 0.5;
dr = uniformDR(scale);
pisFactory = pi3dFactory(dr, cellsFactory,
    @parallelepipedIntervalContainer);
% set shape function
shapeFunc = shape3dFunction('x + y');
boundaries = boundaryIntervals3d(
    boundaryInterval(3, 15),
```

```

    boundaryInterval(3, 10),
    boundaryInterval(10, 60));
pfContainer = parallelepipedPFContainer(boundaries);
% build porous function
pf1 = pf3d(shapeFunc, pisFactory, pfContainer);

% pf2
% set cell type
cellData = ellipsoidCellData(1, 1, 1);
cellsFactory = cells3dFactory(cellData, @bbox3d);
% set porous intervals factory
scale = 0.3;
dr = uniformDR(scale);
pisFactory = pi3dFactory(dr, cellsFactory,
    @parallelepipedIntervalContainer);
% set shape function
shapeFunc = shape3dFunction('x^2 + y');
boundaries = boundaryIntervals3d(
    boundaryInterval(5, 12),
    boundaryInterval(5, 15),
    boundaryInterval(12, 50));
pfContainer = parallelepipedPFContainer(boundaries);
% build porous function
pf2 = pf3d(shapeFunc, pisFactory, pfContainer);

```

FIG. 7.1: Shape addition of F_p^1 and F_p^2

It is important to note that the shape addition is a commutative operation only in terms of *equality* (Def. 6.1) only if both porous functions have the same distribution rule and cell type.

Although in general the shape addition is not commutative, it describes the natural situation of adding two different porous (or granular) materials.

7.2. Body addition. Another type of addition [1]) is the body addition. It is somewhat similar to a point-wise addition of matrices. The main idea

is to fill the empty space of the first porous function by the cells of the second porous function.

Consider F_p^1 and F_p^2 :

$$F_p^1 = \{I_{p_i}^1\}_{i \in I^1}, \quad (7.6)$$

$$F_p^2 = \{I_{p_i}^2\}_{i \in I^2}, \quad (7.7)$$

DEFINITION 7.2. Body addition $\cup^b$ of F_p^1 and F_p^2 is defined as

$$F_p^1 \cup^b F_p^2 = \{I_{p_i}^1 \cup^b I_{p_i}^2\}_{i \in I^1 \cup^b I^2}, \quad (7.8)$$

$$I^1 \cup^b I^2 = I^1, \quad (7.9)$$

$$I_{p_i}^1 \cup^b I_{p_i}^2 = \{C_j\}_{j \in J^1} \cup^b \{C_j\}_{j \in J^2} = \{C_j\}_{j \in J^1 \cup (J^2 \setminus J^1) \cup \Phi(J^1 \cap J^2)}, \quad (7.10)$$

where $\Phi(J)$ is a relation producing the closest unused index (used for the cells of the second addend, whose corresponding locations in the first addend are taken).

In Fig. 7.2 the result of the body addition of two porous functions is shown for the same functions as in Section 7.1.

FIG. 7.2: Body addition

8. Subtraction of Porous Functions

The main idea of subtracting one porous function from another consists of removing some cells of one porous function from the other. This operation is similar to the set difference ($\setminus$).

DEFINITION 8.1. For F_p^1 defined by (7.6) and F_p^2 defined by (7.7)

$$F_p^1 - F_p^2 = F_p^1 \setminus F_p^2 = \{I_{p_i}^1 \setminus I_{p_i}^2\}_{i \in I^1 \setminus I^2}. \quad (8.1)$$

The following code snippet illustrates the operation of subtraction of two porous functions, and the result is shown in Fig. 8.1.

```
%% Difference of two porous functions
% pf1
% set cell type
cellData = ellipsoidCellData(1, 1, 1);
cellsFactory = cells3dFactory(cellData, @bbox3d);
% set porous intervals factory
scale = 1;
dr = uniformDR(scale);
pisFactory = pi3dFactory(dr, particlesFactory,
    @parallelepipedIntervalContainer);
% set shape function
shapeFunc = shape3dFunction('x + y');
% create pf1
boundaries = boundaryIntervals3d(
    boundaryInterval(3, 10),
    boundaryInterval(3, 10),
    boundaryInterval(12, 20));
pfContainer = parallelepipedPFContainer(boundaries);
pf1 = pf3d(shapeFunc, pisFactory, pfContainer);
% pf2
% set cell type
cellData = ellipsoidCellData(1, 1, 1);
cellsFactory = cells3dFactory(cellData, @bbox3d);
% set porous intervals factory
scale = 1;
dr = uniformDR(scale);
pisFactory = pi3dFactory(dr, particlesFactory,
    @parallelepipedIntervalContainer);
% set shape function
shapeFunc = shape3dFunction('20');
% create pf2
boundaries = boundaryIntervals3d(
    boundaryInterval(7, 10),
    boundaryInterval(5, 9),
    boundaryInterval(12, 20));
pfContainer = parallelepipedPFContainer(boundaries);
pf2 = pf3d(shapeFunc, pisFactory, pfContainer);
```

Such definition of subtraction satisfies $F_p^1 - F_p^1 = F_p^0$, where F_p^0 is a zero porous function – the height of all its porous intervals is zero.

9. Multiplication by a Scalar

The multiplication of a porous function by a scalar modifies its shape by setting the height of each its porous interval by its replication. For $n \in N$ we have simply

$$n * F_p = \{n * I_{p_i}\}_{i \in I}, \quad (9.1)$$

$$n * I_p = \{C_j\}_{j \in J \cup_{p=1}^n (J+p*h)}. \quad (9.2)$$

FIG. 8.1: Subtraction of porous functions

An example of scalar multiplication of F_p^1 defined in Section 8 by $n = 2$ can be seen on Fig. 9.1.

 FIG. 9.1: Multiplication by a scalar: nF_p^1 for $n = 2$

10. Conclusion

In this paper, we have presented basic operations with porous functions in more detail, and provided necessary computational tools in the form of the Porous Functions Toolbox for MATLAB.

The current implementation of this toolbox allows the creation of porous functions of one and two variables, with various constraints, with various distribution laws/rules (uniform, normal distribution, etc.) defining positions of grains/pores of a porous function, with cells of various shapes and sizes for placement of grains and pores.

The Porous Functions Toolbox is based on the object-oriented programming paradigms, allowing for easy extension and customization of the existing functionality.

The main purpose of the Porous Functions Toolbox is to provide an easily understandable and flexible tool for modeling the structure of various real-world materials (porous, granular, composite, ...) and for performing basic operations with porous functions for their applications in science and engineering.

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BERG Faculty, Technical University of Kosice
B. Nemcovej 3
04200 Kosice, SLOVAKIA

e-mail: iryna.trymorus@tuke.sk;
igor.podlubny@tuke.sk

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