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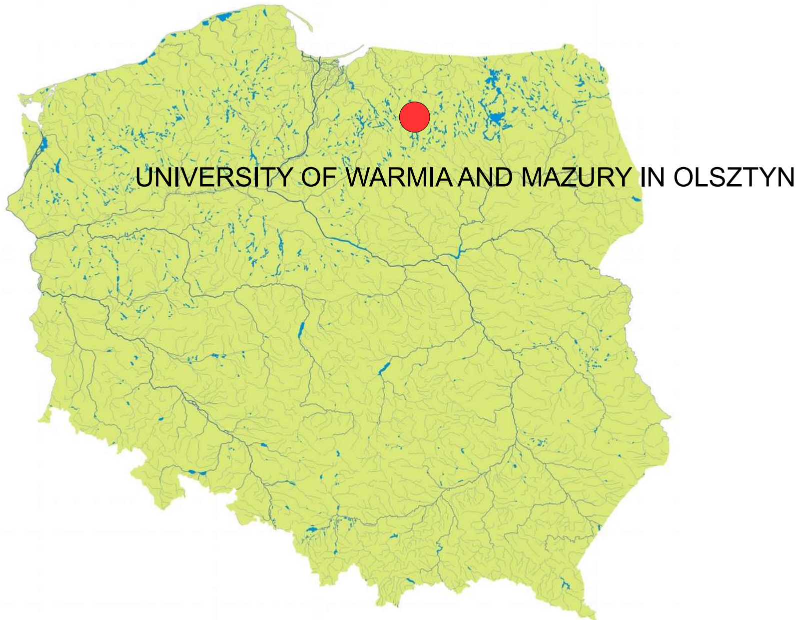
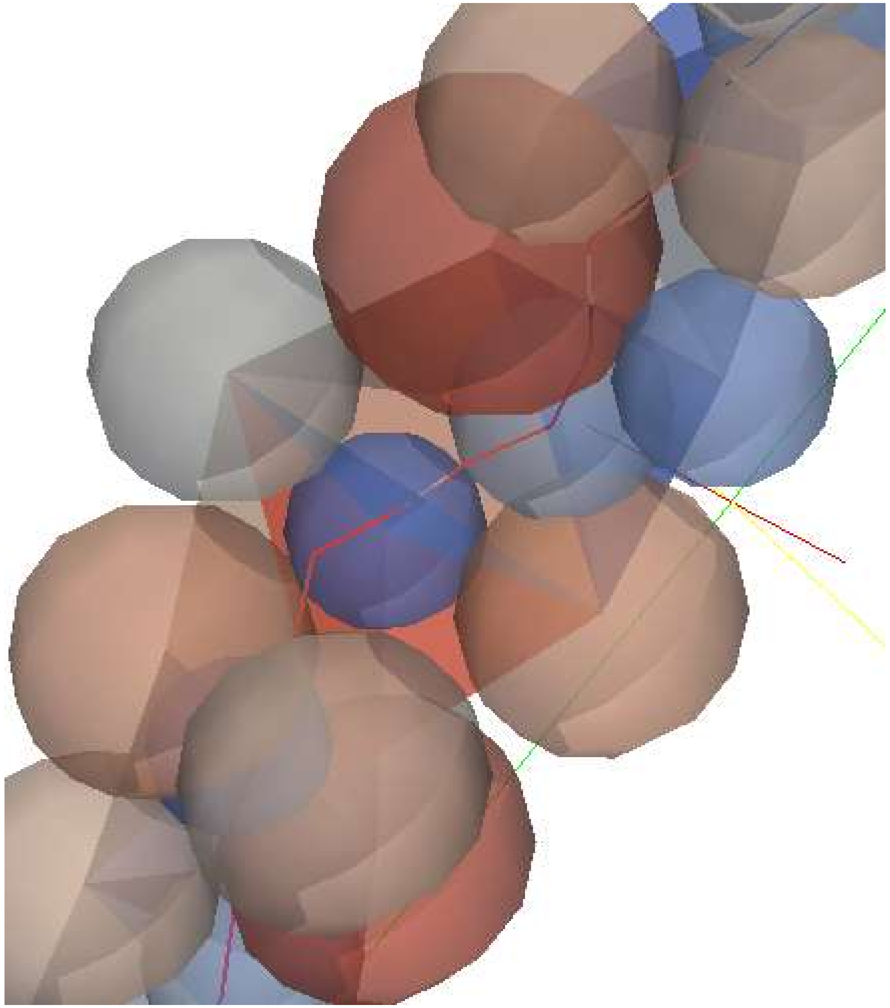
Path Tracking Method

Wojciech Sobieski



Path Tracking Method (PTM) – iterative method of determination of the length of pore channel in the chosen space direction, which consists in analyzing the local structure of the pore space based on vector geometry.

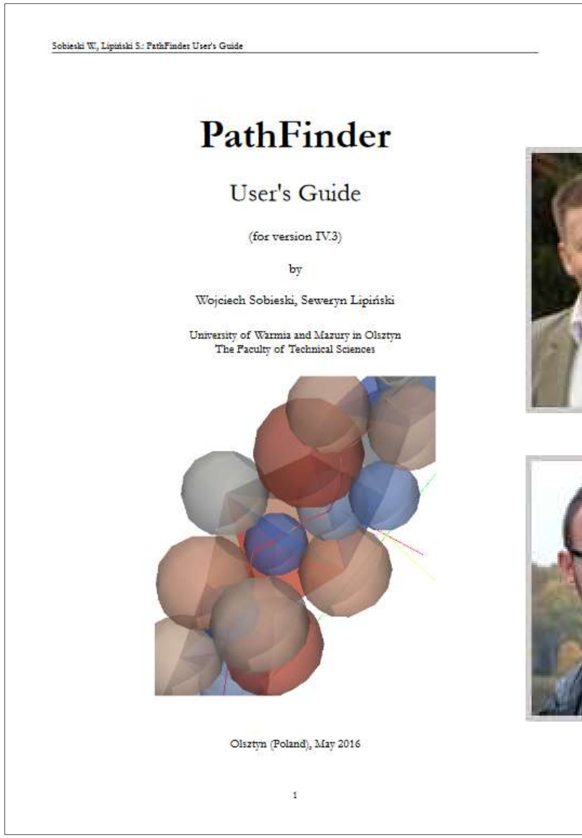


PTM was developed in order to calculate the **geometric tortuosity** of a granular bed.

PTM is implemented in **PathFinder code,** which was written on my own.

PathFinder – a program destined for the analysis of the spatial structure of granular beds or its parts, of a cylindrical or cubical shape. The program is available free of charge with source code and can be used on Windows or Unix/Linux.

PathFinder needs additional software to work: gfortran compiler (for compiling source code), the Gnuplot environment (for basic visualization and analysis of the calculations) and ParaView or MayaVi (for the visualization and analysis of results).


Sobieski W., Lipiński S.: PathFinder User's Guide

PathFinder

User's Guide

(for version IV.3)

by

Wojciech Sobieski, Seweryn Lipiński

University of Warmia and Mazury in Olsztyn
The Faculty of Technical Sciences

Olsztyn (Poland), May 2016

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Sobieski W., Lipiński S.: PathFinder User's Guide [on-line].
URL: http://www.uwm.edu.pl/pathfinder/index.php
University of Warmia and Mazury in Olsztyn (Poland), 2013.

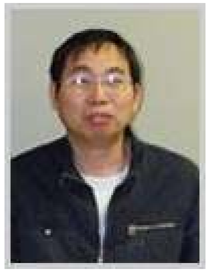
Wojciech Sobieski developed PTM for granular beds in 2009 during an internship at the University of Manitoba in Winnipeg.

The inspiration to start the work on the method was the observation that DEM simulation results can be used to analyze the internal structure of porous media, in particular for the calculation of various geometrical parameters, including tortuosity.

DEM – Discrete Element Method

University of Manitoba (Winnipeg, Canada)

Qiang Zhang



Chuanyun Liu

Sobieski W.: http://pracownicy.uwm.edu.pl/wojsob/ (in Polish)

In **2009**, the first working version of the program was created; the process of its creation was described in the Research Report No 1/2009 (in Polish).

In the first phase of the project, the determination of **geometric tortuosity** in porous media was investigated; then other features were added.

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Telephone (204) 474-6033
Fax (204) 474-7512

March 29, 2010

To Whom It May Concern:

This is to confirm that Dr. Wojciech Sobieski worked as a Research Associate from September 18, 2009 to March 17, 2010 in the Department of Biosystems Engineering, University of Manitoba, Canada. He was involved in a research project entitled "Pore Structure and Airflow Resistance of Bulk Solids". He has developed an algorism to calculate the tortuosity for airflow through porous beds, and conducted experiments to measure the resistance to airflow through a porous bed.

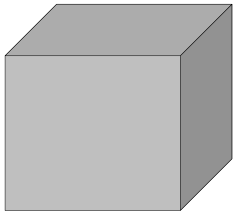
Sincerely,

Qiang Zhang, PEng, PhD
Professor and Acting Associate Dean (Research)

Sobieski W.: Calculating tortuosity in a porous bed consisting of spherical particles with known sizes and distribution in space (in Polish). Research report 1/2009, Winnipeg (Canada), 2009.

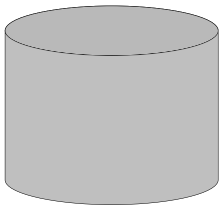
The main data calculated in the PathFinder code:

Bed volume (when a cuboid domain is analyzed)



$$V_d = (x_{max} - x_{min}) \cdot (y_{max} - y_{min}) \cdot \left[z_{n_s - n_{s\_rej}} + 0.5 \cdot d_{n_s - n_{s\_rej}} - z_{min} \right]$$

Bed volume (when a cylindrical domain is analyzed)



$$V_d = \frac{\pi \cdot d_{cyl}^2}{4} \cdot \left[z_{n_s - n_{s\_rej}} + 0.5 \cdot d_{n_s - n_{s\_rej}} - z_{min} \right]$$

$$d_{cyl} = \frac{1}{2} \cdot \left[(x_{max} - x_{min}) + (y_{max} - y_{min}) \right]$$

Total volume of the solid body:

$$V_s = \sum_{i=1}^{n_s - n_{s\_rej}} \frac{1}{6} \cdot \pi \cdot d_i^3$$

Inner surface of the solid body:

$$S_p = \sum_{i=1}^{n_s - n_{s\_rej}} \pi \cdot d_i^2$$

Specific surface of the porous body:

$$S_{0,Kozeny} = \frac{S_p}{V_d} \qquad S_{0,Carman} = \frac{S_p}{V_s}$$

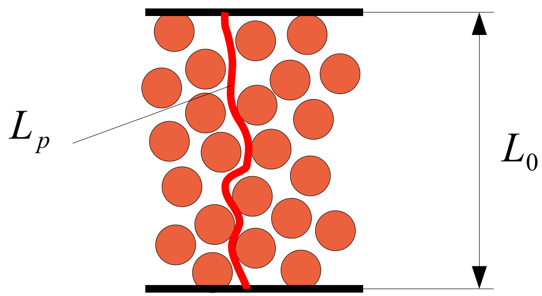
Porosity:

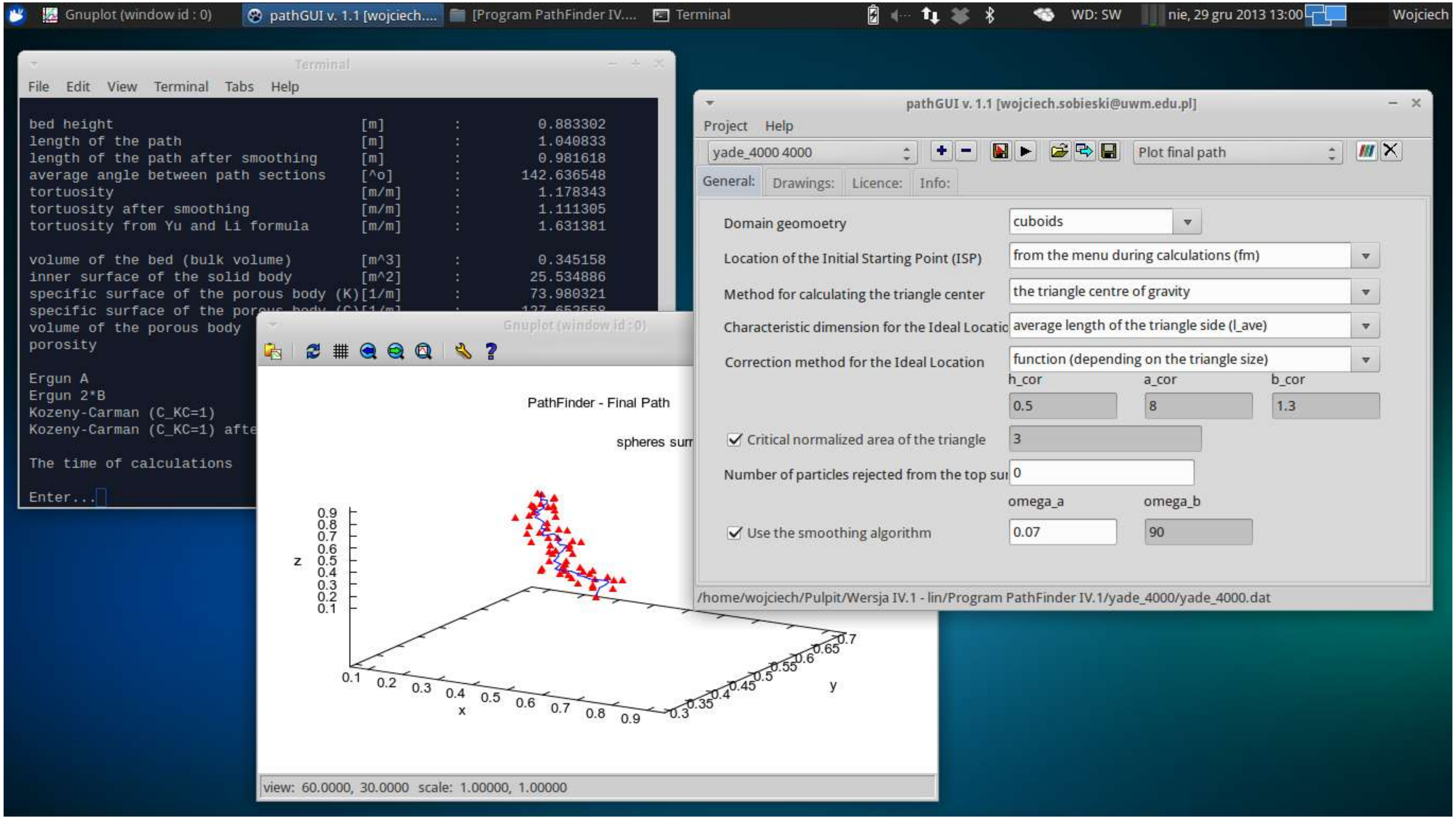
$$\phi = 1 - \frac{V_s}{V_d}$$

PTM is applied here

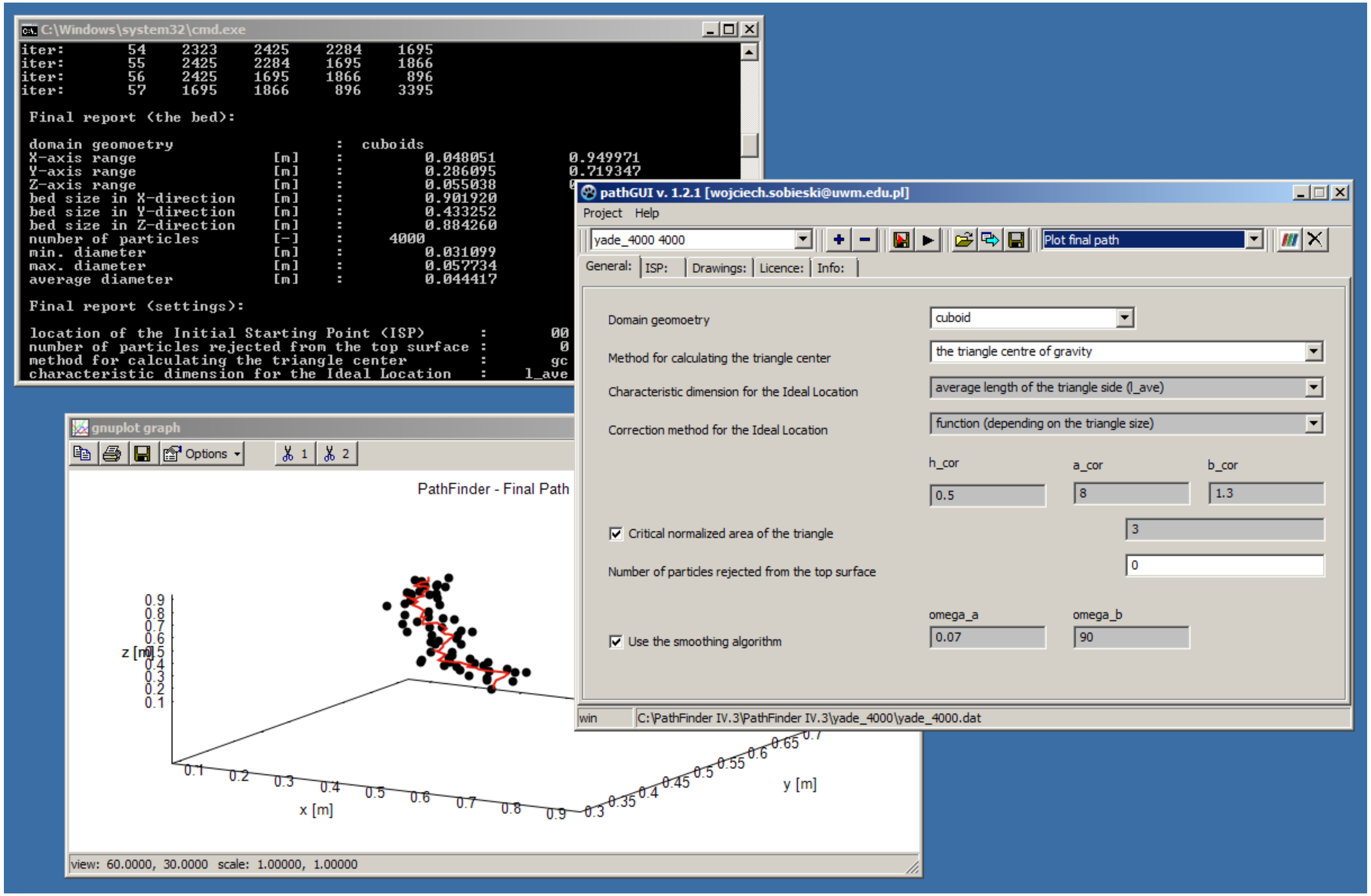
Geometric tortuosity:

$$\tau = \frac{L_p}{L_0}$$





PathFinder v. 1.1 in Linux (xUbuntu)



PathFinder v. 1.2.1 in Windows

Currently the **PathFinder code** is available on the Internet. On the project page, interested Reader can find more information, as well as download the source code and additional tools.

www.uwm.edu.pl/pathfinder

PathFinder - a program destined for analysis the spatial structure of granular beds, or its parts, of a cylindrical or cubical shape (Fig. 1). The program is available free of charge with source code and can be used on Windows or Unix/Linux. The program needs additional software to work: gfortran compiler (for compiling source code), the Gnuplot environment (for basic visualization and analysis of the calculations) and ParaView (for the visualization and analysis of results). These programs are also available free of charge under the GPL license for both Windows and Unix/Linux.

Path Tracking Method (PTM) - iterative method of determination of the length of pore channel in the chosen space direction, which consists in analyzing the local structure of the pore space based on vector geometry.

In the case of Pathfinder code, the length of pore channel is determined between two parallel planes based on the sum of the unitary lengths, calculated based on so-called tetrahedral structures, which establish the basis for the calculation algorithm. Tetrahedral structures are created based on the data on the location and diameter of each particle in the bed. The data for calculations are obtained from DEM simulation or from the analysis of a set of tomography scans. Details concerning method are available in the User's Guide.

Wojciech Sobieski developed PTM for granular beds in 2009 during an internship at the University of Manitoba in Winnipeg (see the official confirmation). The inspiration to start work on a method was observation, resulting from the author's extensive experience in programming, that DEM simulation results can be used to analyze the internal structure of porous media, in particular for the calculation of various geometrical parameters, including tortuosity. In 2009, the first working version of the program was created; the process of its creation was described in the Research Report No 1/2009. This report later became the basis for several articles in peer-reviewed journals.

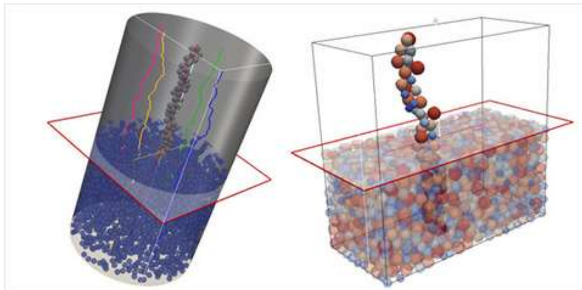
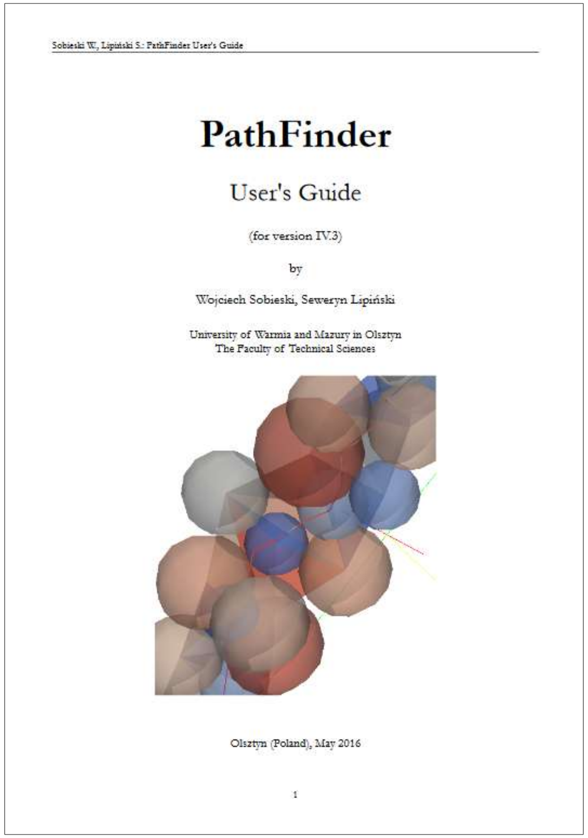


Fig. 1 Examples of visualization of the results of calculations performed with the use of PathFinder program.

Wojciech Sobieski – web designer
Dariusz Grygo – web designer (in the past)

Before using the **PathFinder code** (or other elements of the **PathFinder Project**), please read the licence.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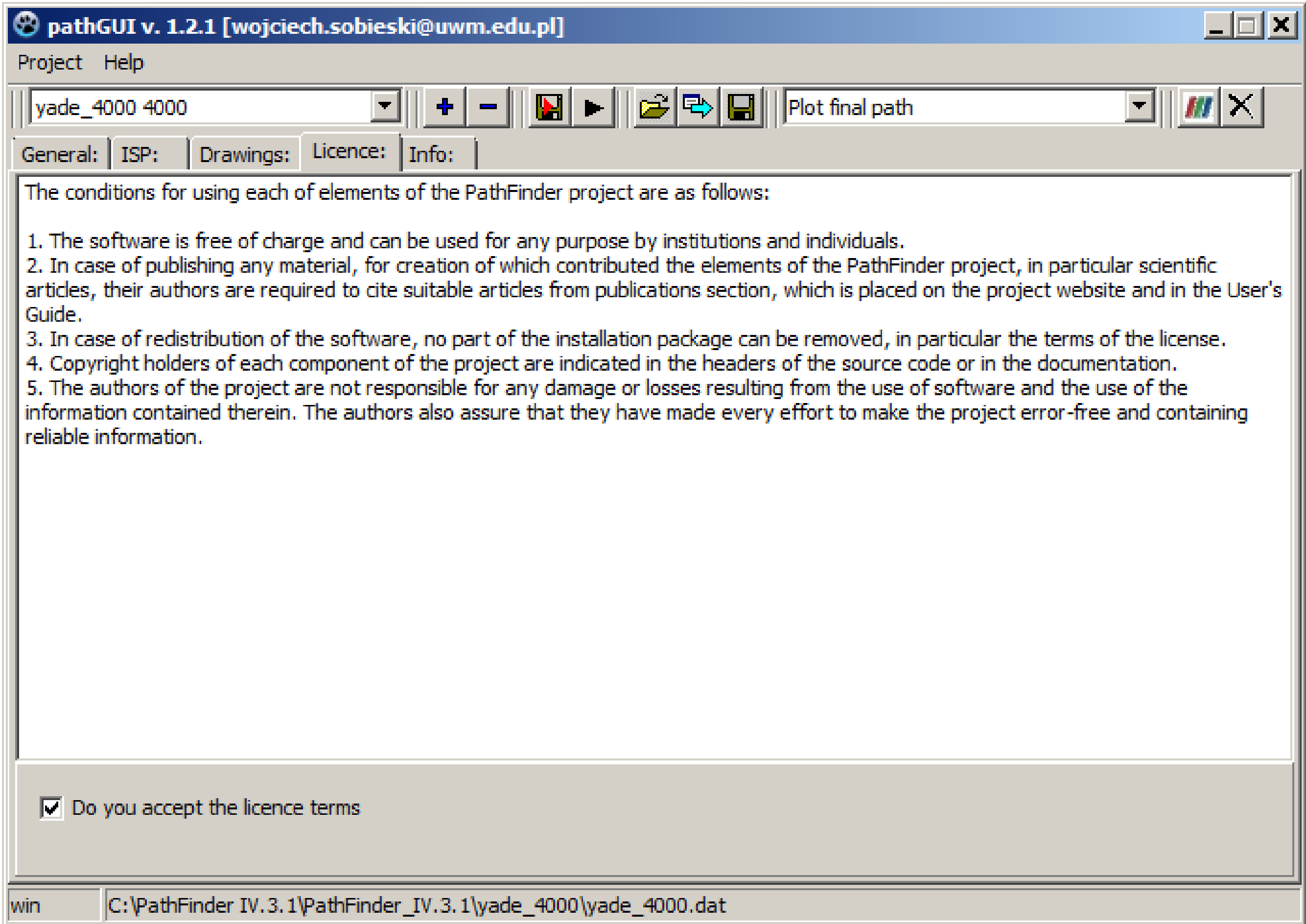

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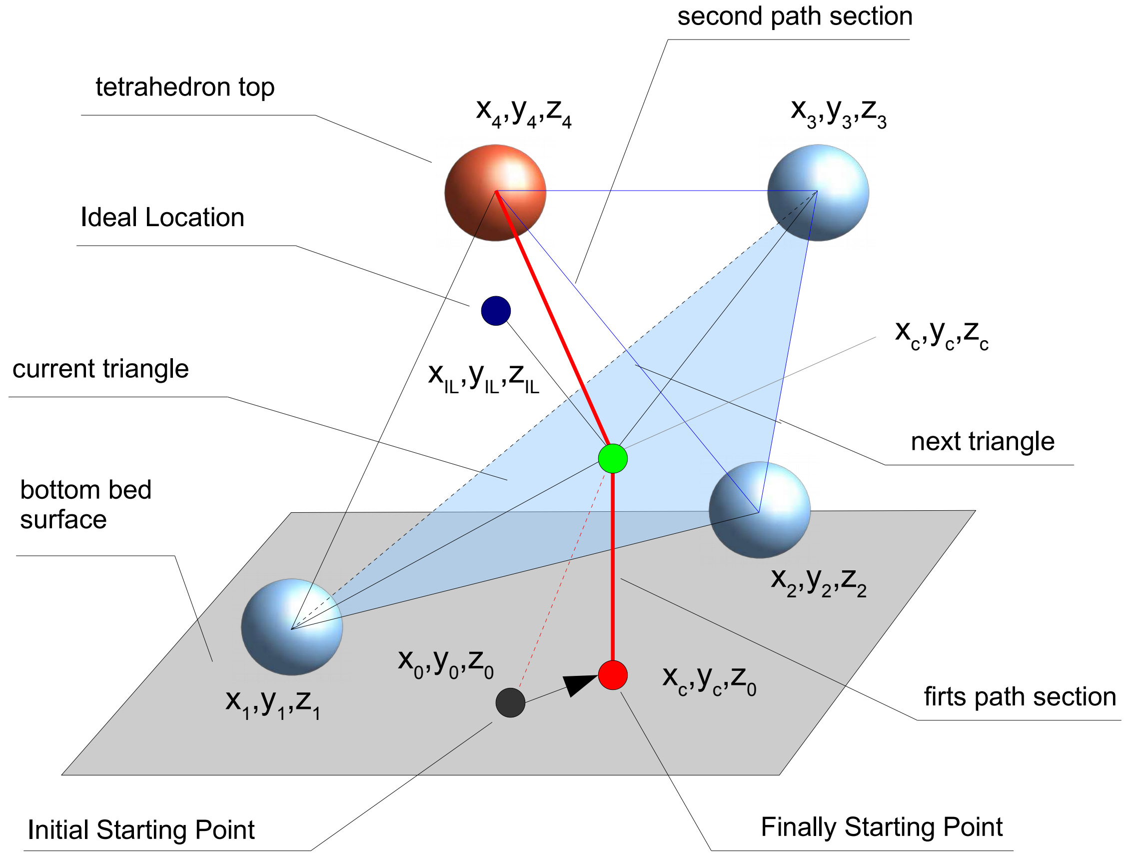
PTM Algorithm

The length of pore channel L_p is determined between two parallel planes based on the sum of the unitary lengths, calculated based on so-called **tetrahedral structures**, which establish the basis for the calculation algorithm.

Tetrahedral structures are created based on the data on the location (x_i, y_i, z_i) and diameter (d_i) of each particle (n_i) in the bed.



$$n_i, x_i, y_i, z_i, d_i$$

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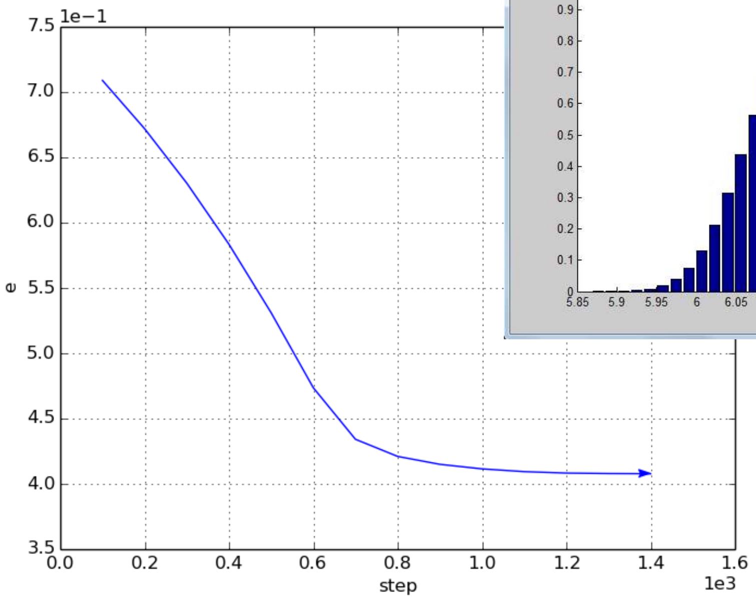
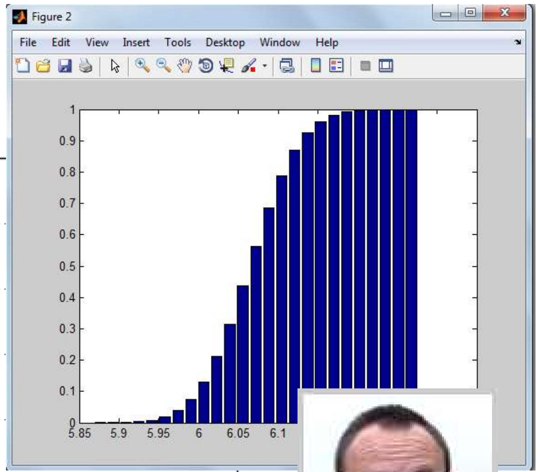
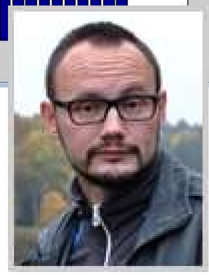
The so-called **indirect way** of obtaining data for the PathFinder code (in cooperation with S. Lipiński)

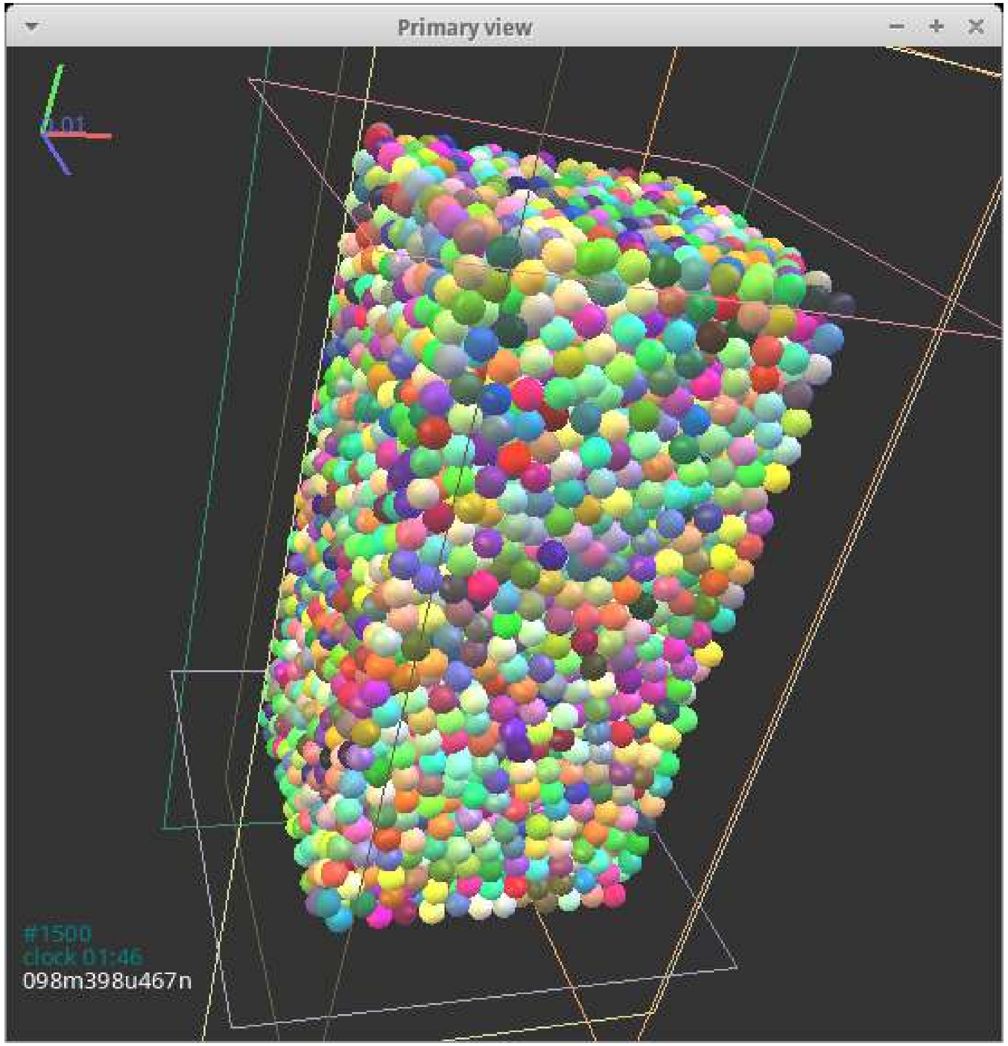
Cumulative curve of particle size distribution

Changes of the porosity during the simulation (Radius Expansion Method)









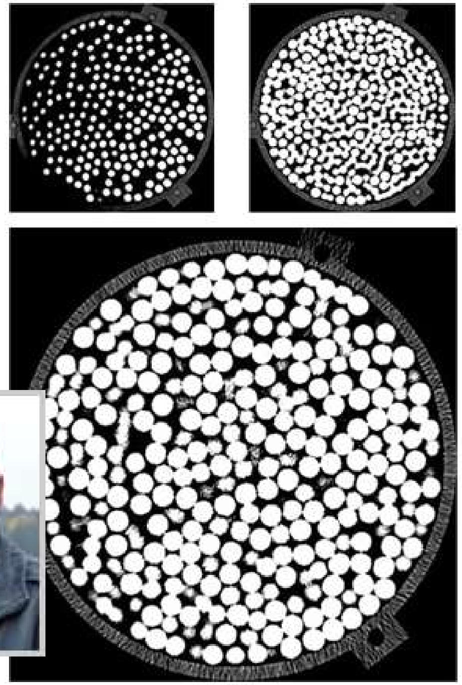
$$n_i, x_i, y_i, z_i, d_i$$

An example of a virtual bed (YADE)

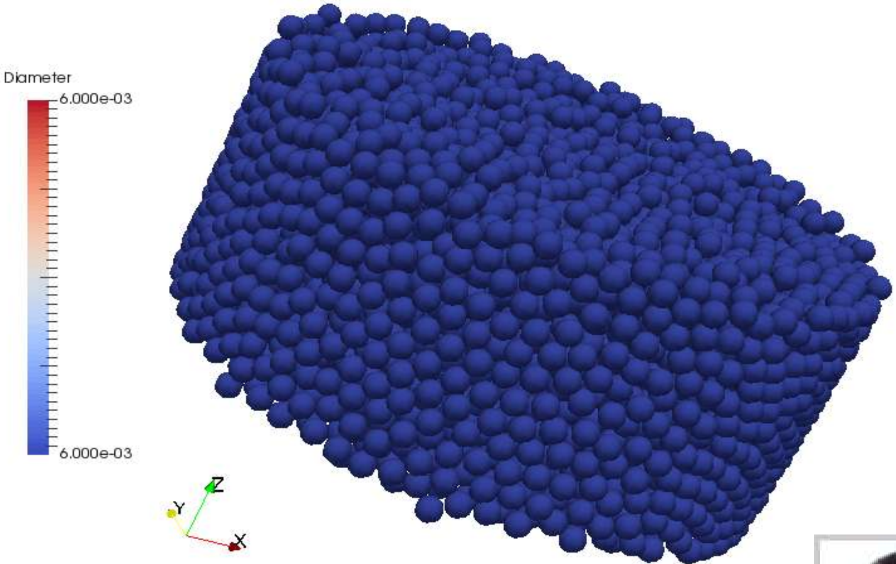
The so-called **direct way** of obtaining data for the PathFinder code (in cooperation with S. Lipiński)

Medical tomograph used in the investigations

Image analysis (particle detection)



Sample of a real granular bed



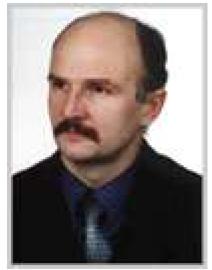
Visualization of the results

$$n_i, x_i, y_i, z_i, d_i$$

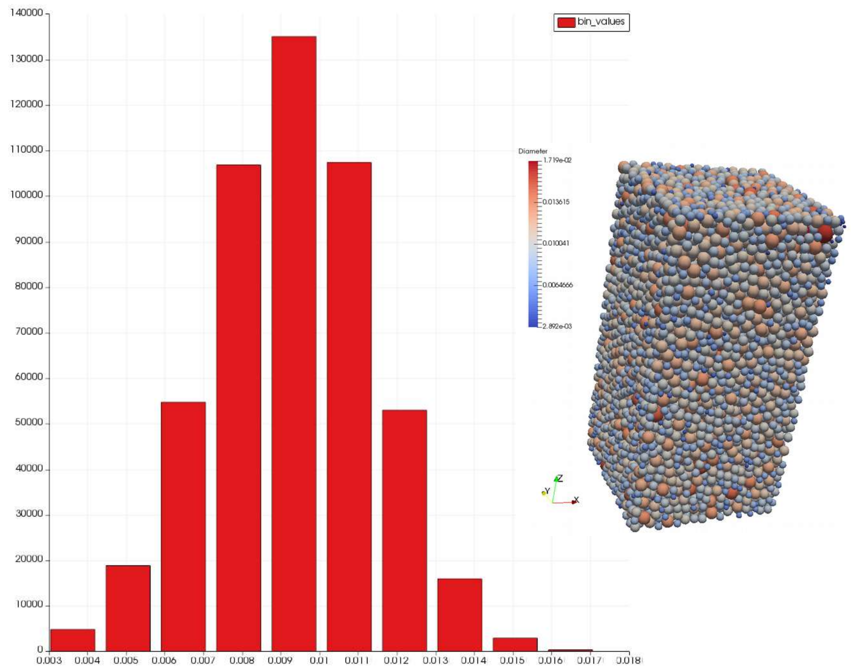
PTM was developed for the analysis of real beds, thus it has some limitations:

- variance of the spheres size distribution cannot be too high – tests have shown (using a bed of beads having an average diameter of 6 [mm]) that the program works properly for variations not higher than 1.1 [mm].

Seweryn Lipiński



Zenon Syroka



An example of the deposit
with a maximum possible variance

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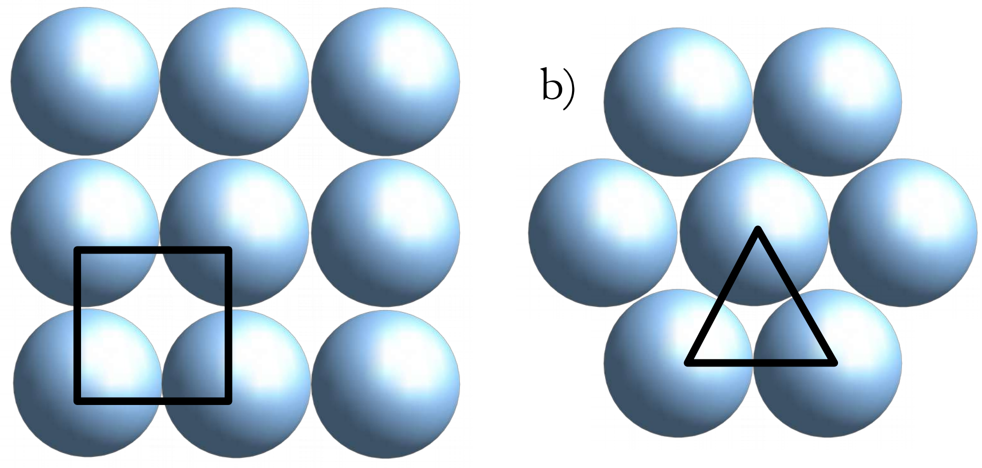
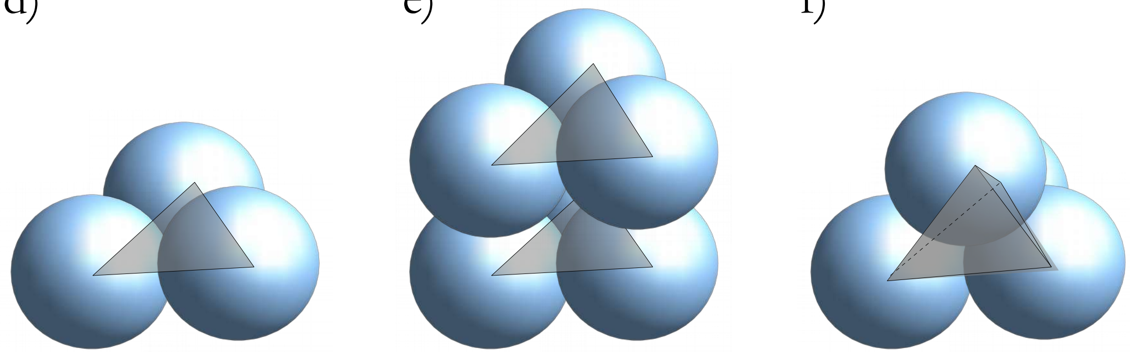
PTM Algorithm – details

a) b)



c)

d) e) f)



Assumption: The basic form of the spatial structure of the bed consisting of spherical particles is a tetrahedron (case f).

Steps: →

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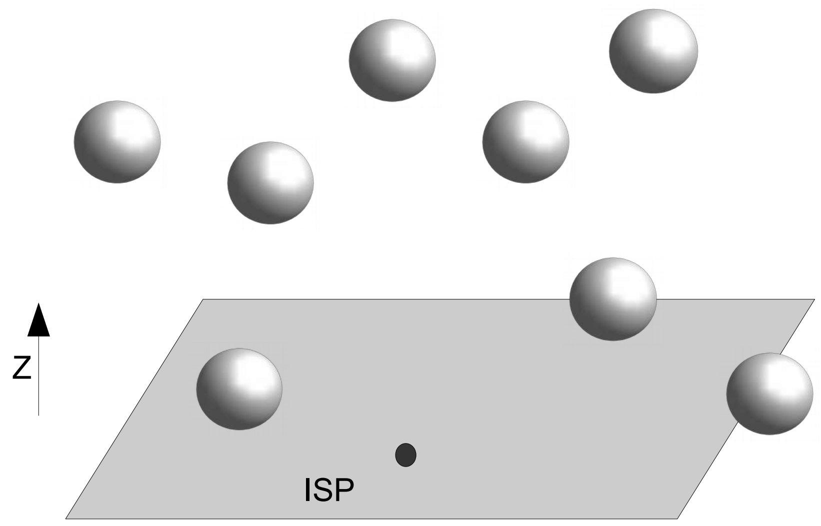
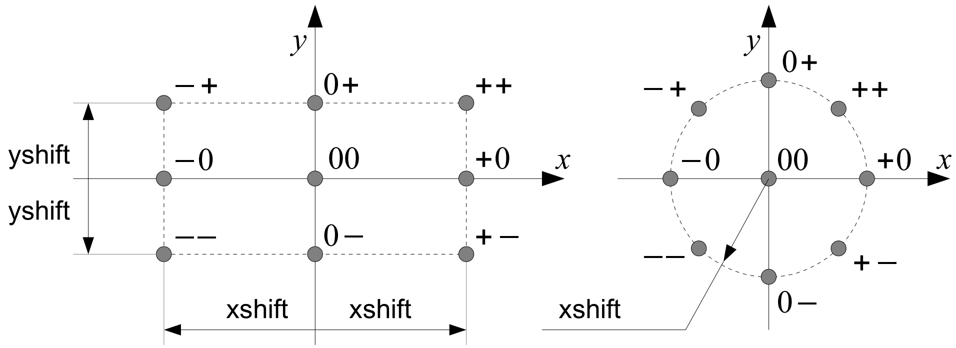
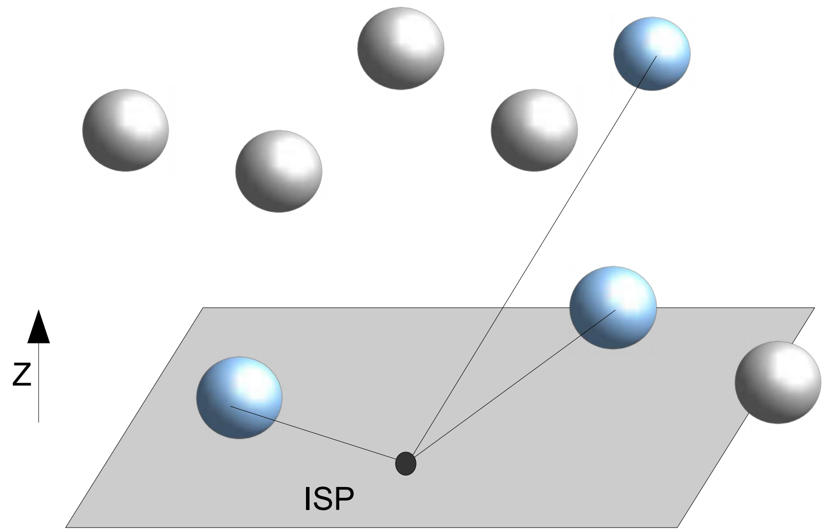


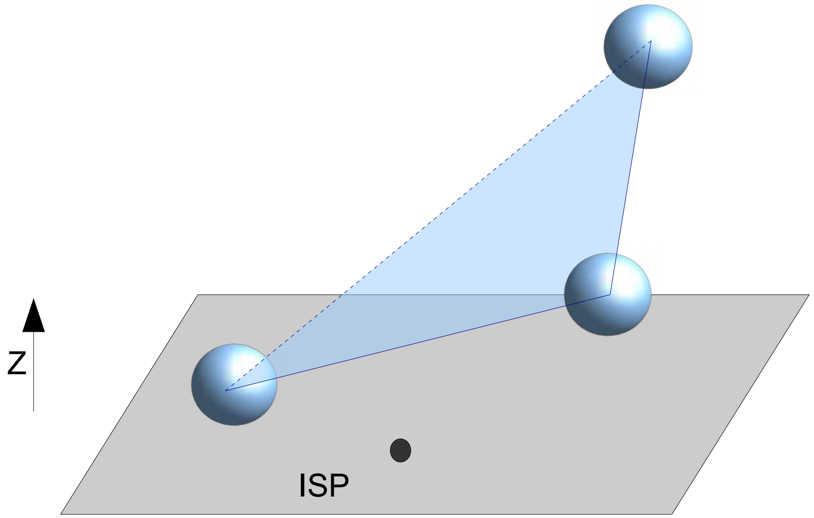
Arbitrarily choose an Initial Starting Point (ISP) at the bottom of the porous bed.





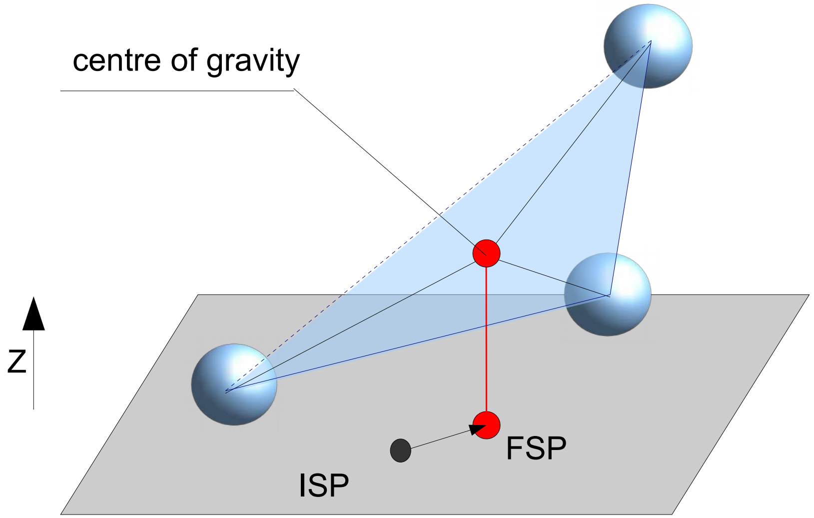
Find three nearest particles to the ISP.

Note: spheres are not in scale.

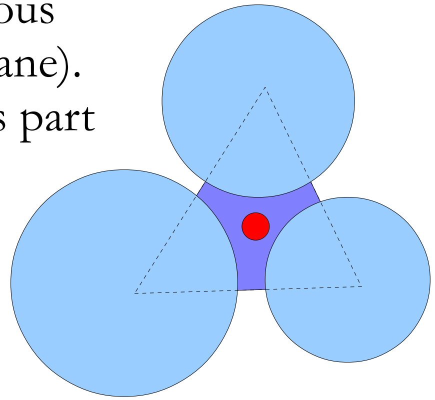


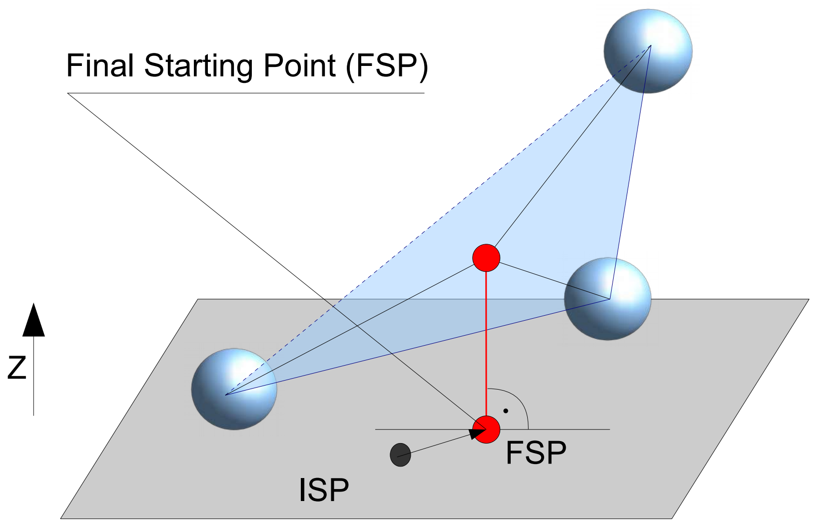
Save information about the first triangle (this will be the basis for the first tetrahedron).

Waldemar Dudda

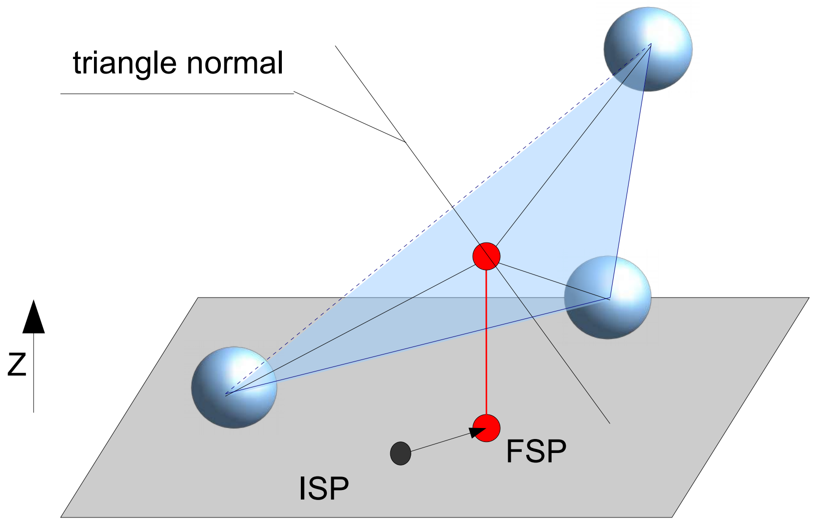


Calculate the coordinates of the centre of gravity of the surface lying in the porous space (in the triangle plane). W. Dudda modified this part in 2016.





Move the Initial Starting Point to the Final Starting Point (FSP) – in this way the first path section is perpendicular to the bottom surface of the bed.



Calculate the normal to the triangle, in the direction of Z axis.

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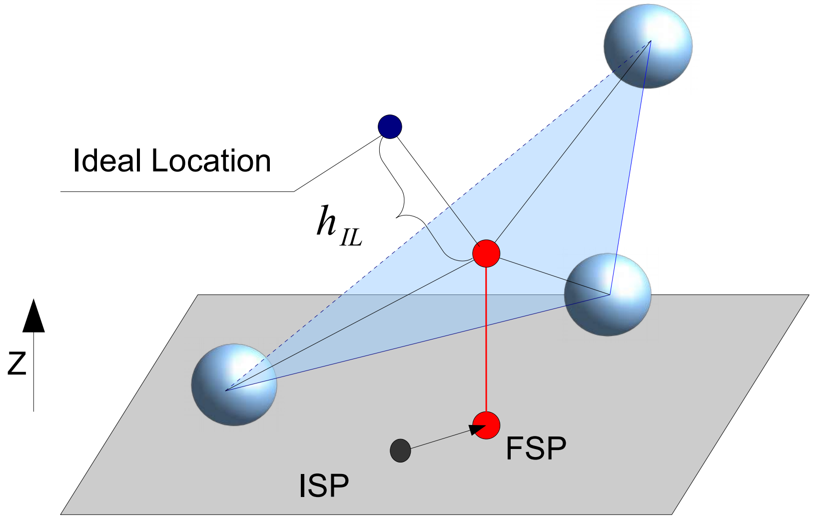
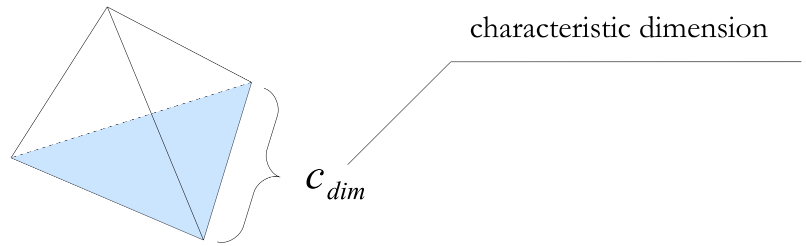
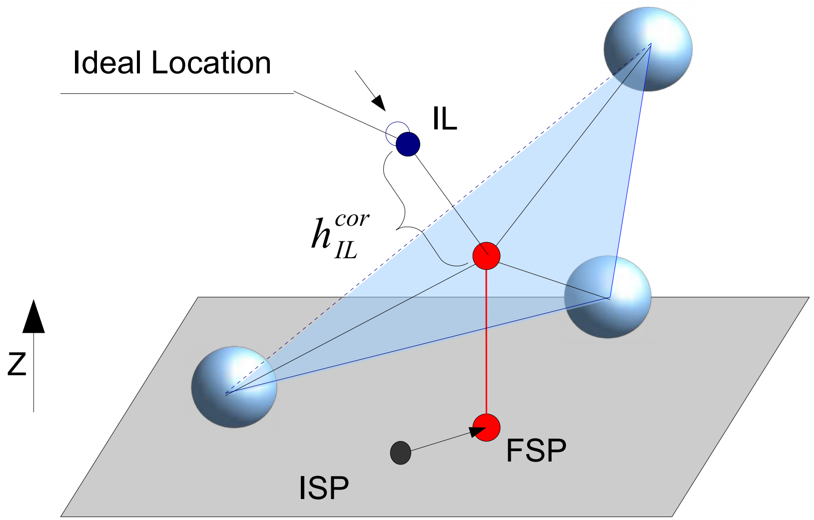
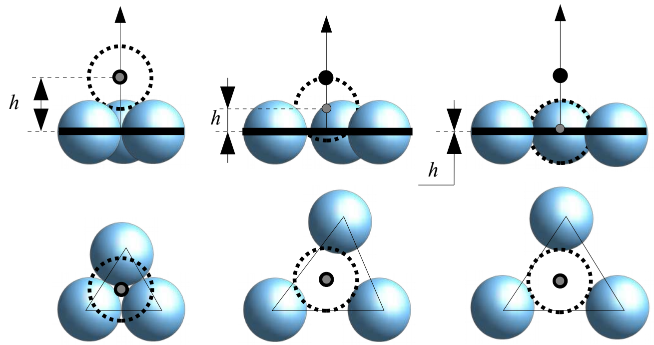


Estimate coordinates of so called Ideal Location (IL), in which should be located the next sphere surrounding the path.





Move the Ideal Location closer to the triangle plane (due to the fact, that particles forming the triangle basis may be separated and in such case the fourth particle is located closer to the triangle plane).



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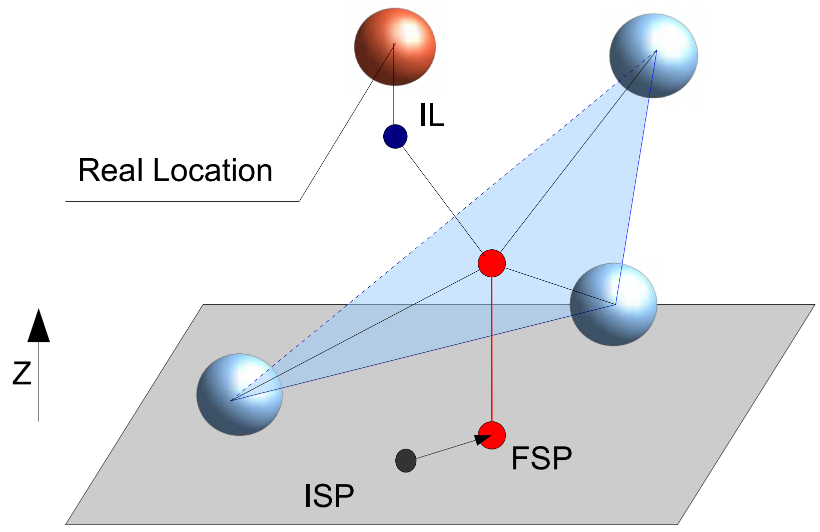
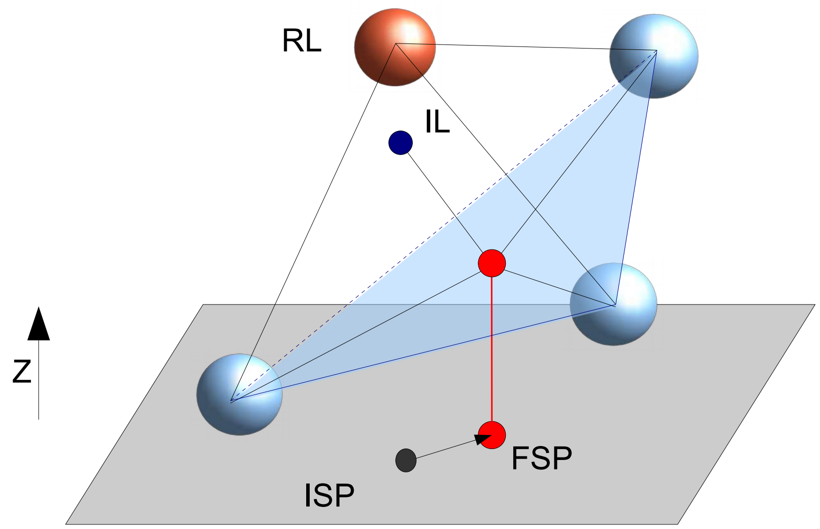
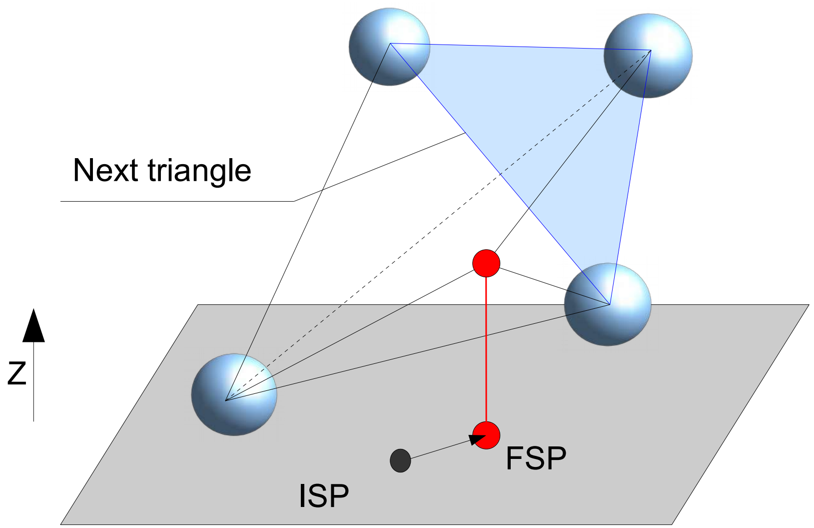


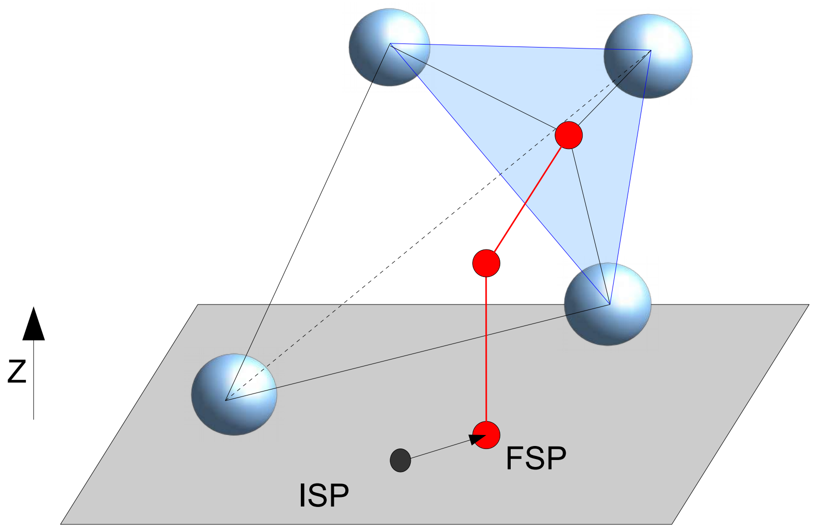
Find the nearest particle to the Ideal Location – this is the Real Location (RL) of the 4-th particle forming tetrahedron in the space.



Save information about the first tetrahedron.



Remove the lowest sphere from tetrahedron 1-2-3-4 to obtain the base triangle for the next tetrahedron.



Continue the calculations, until reaching the top surface of the bed.

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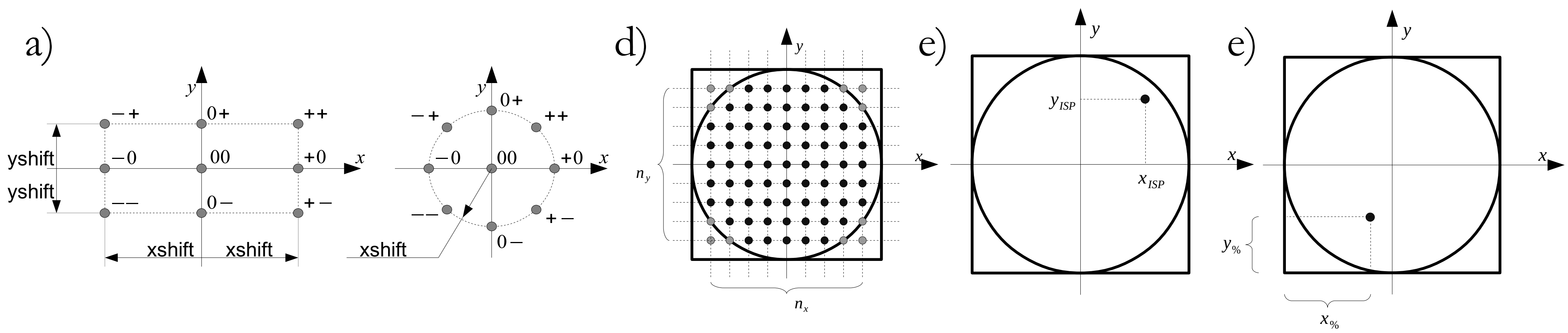
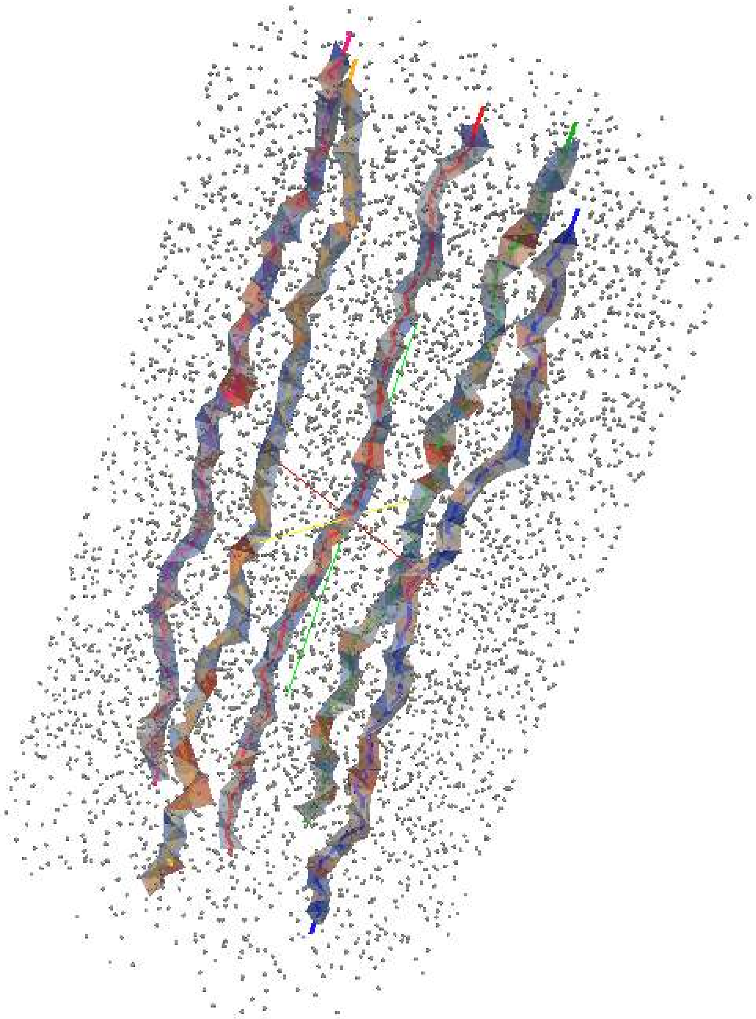
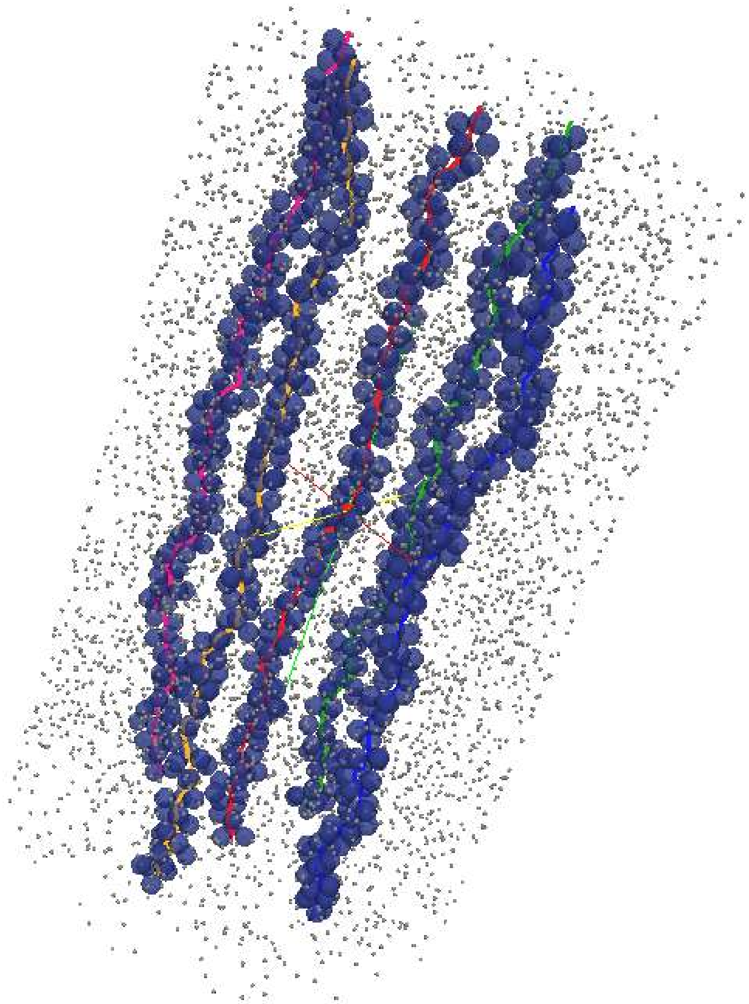
The **Initial Starting Point** (ISP) must be chosen for performing the calculations. Currently such options are available:

a) Choosing ISP directly in the settings file as one of 9 default locations.
b) Choosing ISP after running the program as one of 9 default locations
c) Running calculations for all characteristic Initial Starting Points in one loop.
d) Using the so-called Regular Grid Method.
e) Defining ISP in a file using the "fc" (from coordinates) setting.
f) Defining ISP in a file using the "fp" (from percent) setting.

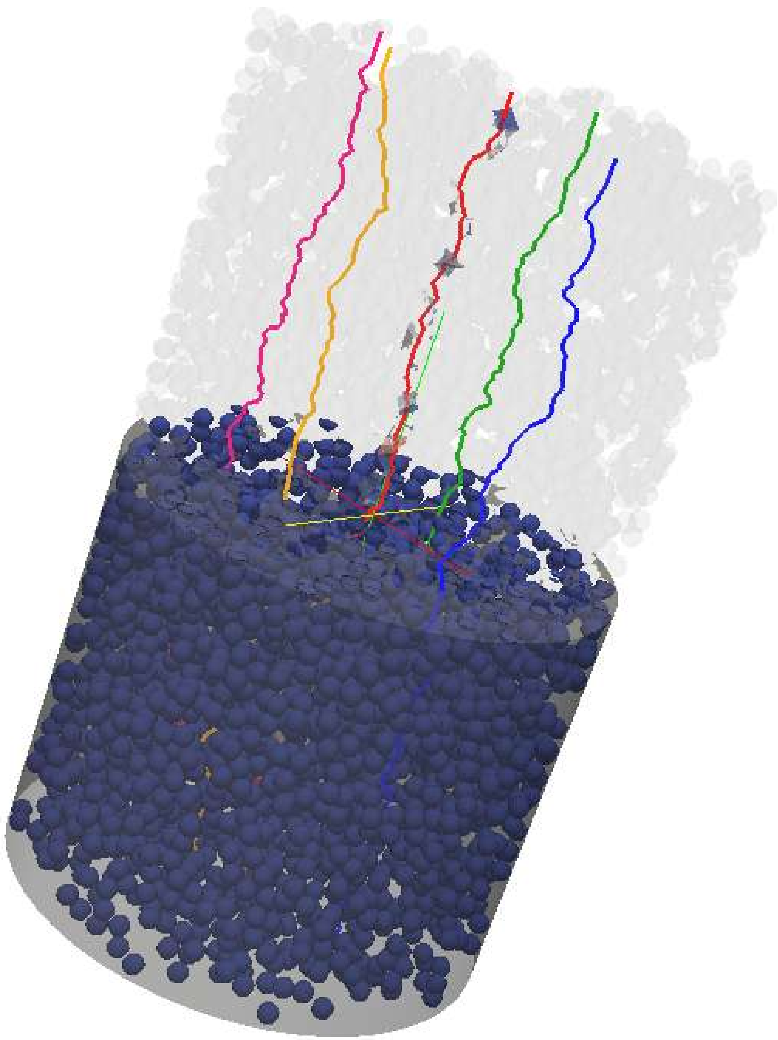




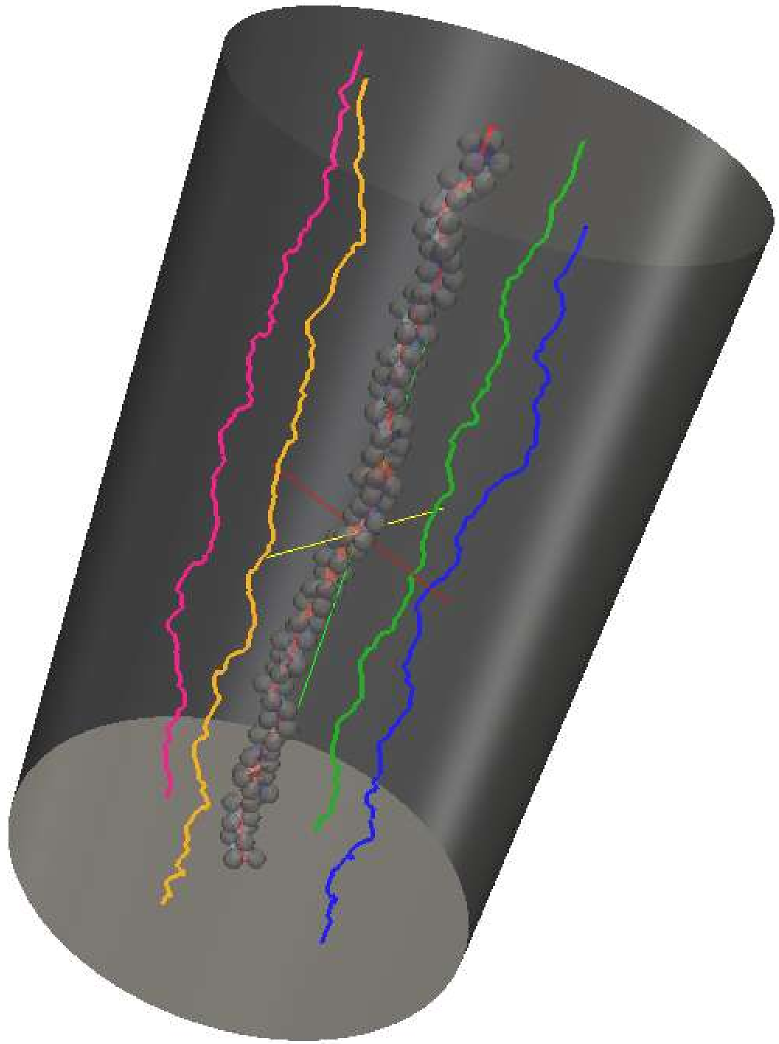
An example of tetrahedral structures in ParaView
(virtual bed created in YADE code)



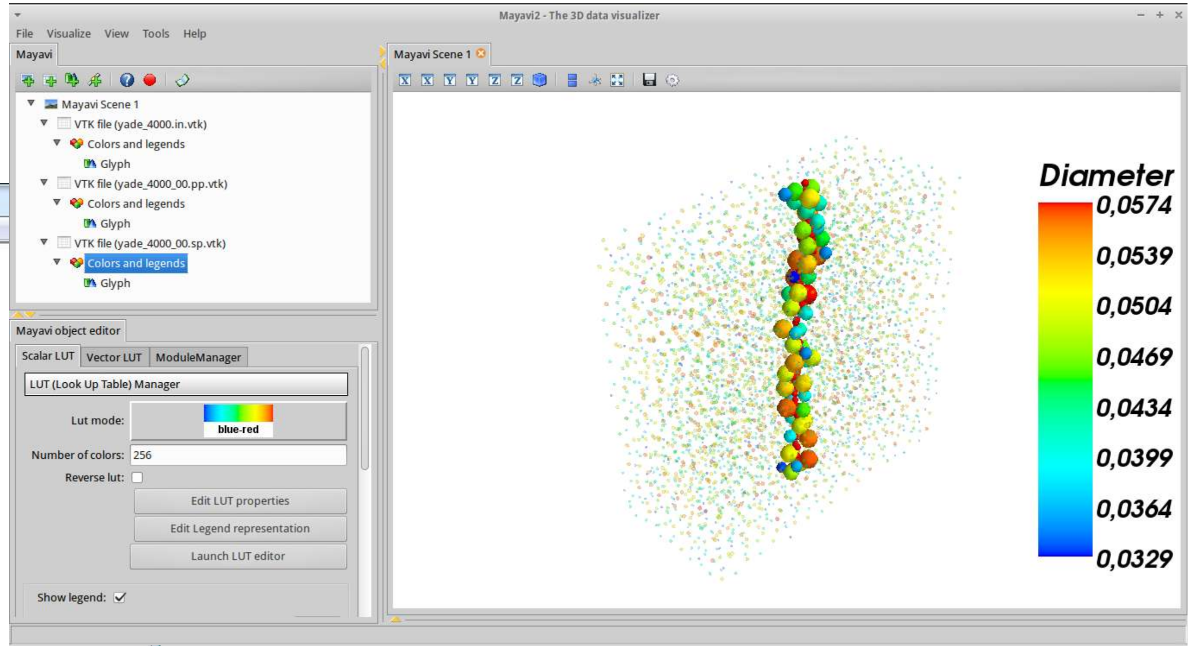
Particles surrounding the paths in ParaView
(virtual bed created in YADE code)



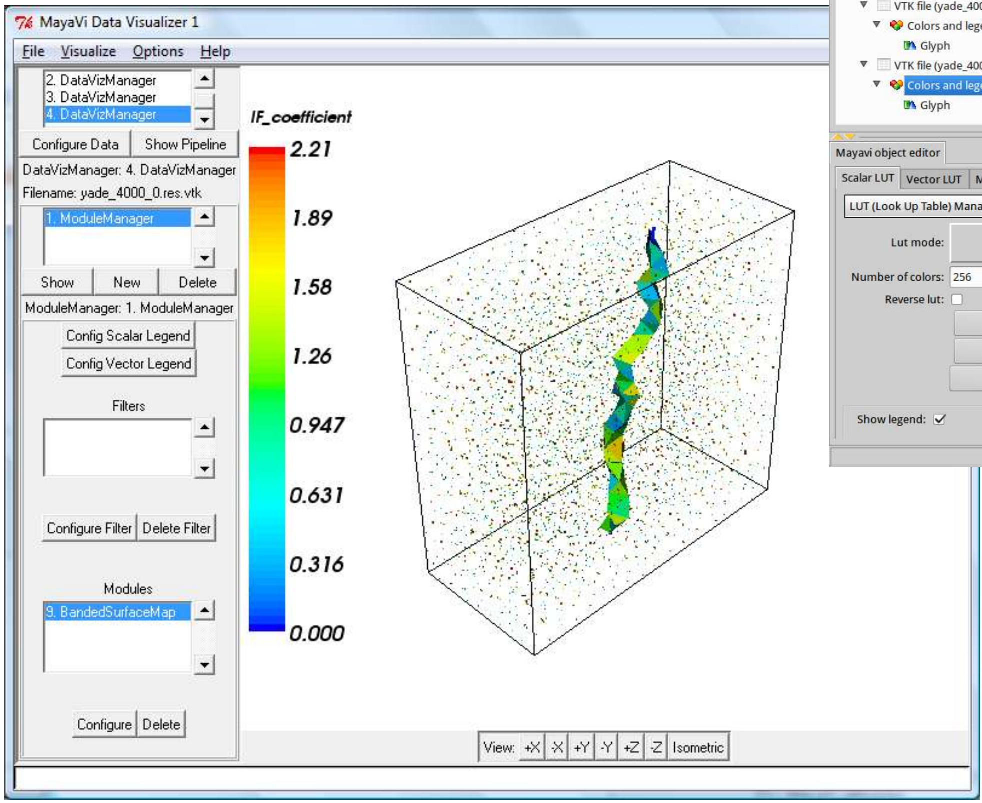
An example of path visualization in ParaView
(virtual bed created in PFC3D code)



An example of path visualization in ParaView
(virtual bed created in PFC3D code)



MayaVi 2.x



MayaVi 1.5

Examples of data visualization
in MayaVi software
(virtual bed created in YADE code)

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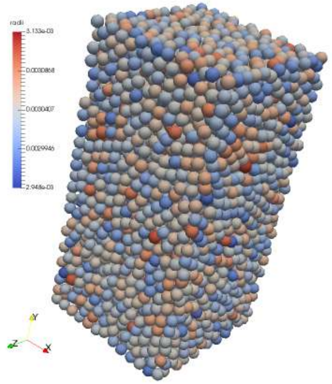
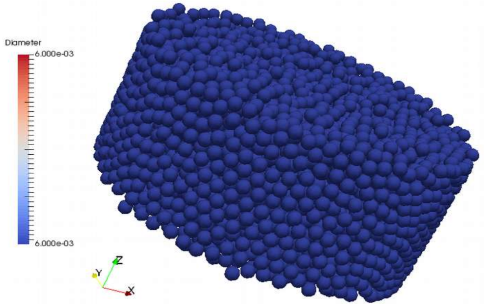
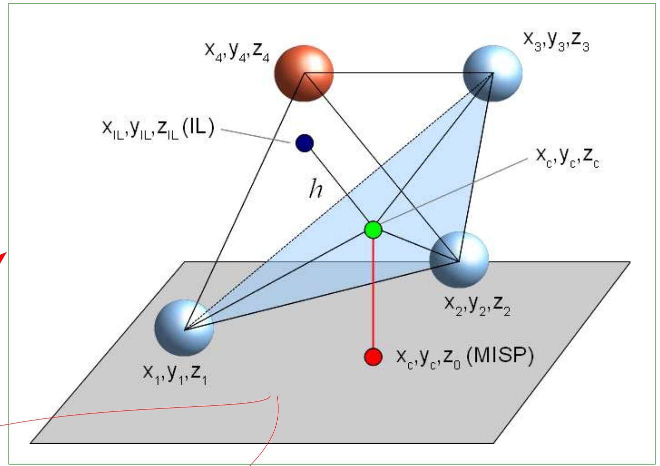




Possibilities of applying the data obtained in the PathFinder code – **analytical approach**

$$n_i, x_i, y_i, z_i, d_i$$

Anna Trykozko



PathFinder

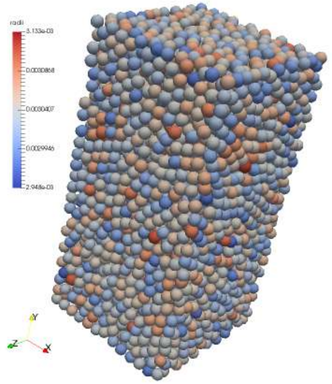
Φ Φ

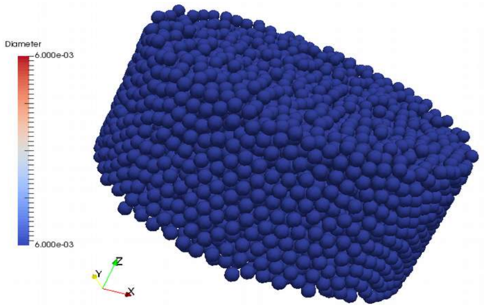
$$\frac{dp}{dx} = A(\Phi)\cdot(\mu \cdot v_f) + B(\Phi)\cdot(\rho \cdot v_f^{\,2})$$

An general formula matching the topology of the Forchheimer equation

$$\Phi = \{d, \phi(V_p, V), \epsilon(V_s, V), e(V_p, V_s), \tau(L_p, L_0), S_0(S_p, V_s, V), \psi(l_x, l_y, l_z)\}$$

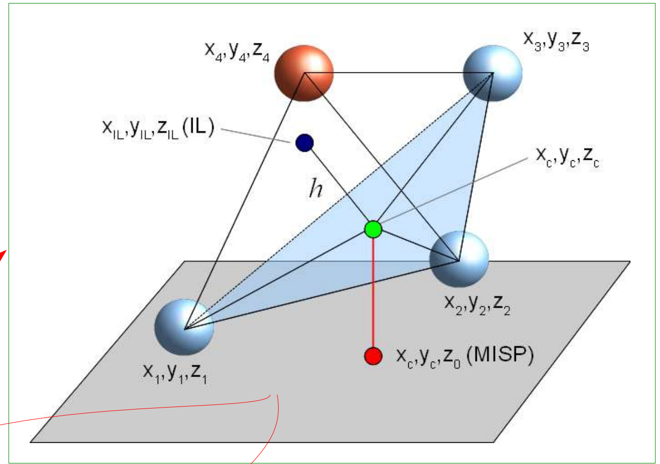
Φ - set of geometrical parameters characterising the spatial structure of a granular bed





Possibilities of applying the data obtained in the PathFinder code – **numerical approach**

$$n_i, x_i, y_i, z_i, d_i$$



PathFinder

Φ Φ

$$\frac{dp}{dx} = A(\Phi)\cdot(\mu\cdot v_f) + B(\Phi)\cdot(\rho\cdot v_f{}^2)$$

Anna Trykozko

$$\frac{\partial}{\partial t}\rho + \nabla(\rho\vec{v}) = 0$$

$$\frac{\partial}{\partial t}(\rho\vec{v}) + \nabla(\rho\vec{v}\otimes\vec{v}) = \nabla(-p\overleftrightarrow{I} + \overleftrightarrow{\tau}) + \rho\vec{s}_b$$

$$\frac{\partial}{\partial t}(\rho e) + \nabla(\rho e\vec{v}) = \nabla((-p\overleftrightarrow{I} + \overleftrightarrow{\tau})\vec{v} + \vec{q}) + \rho s_e$$

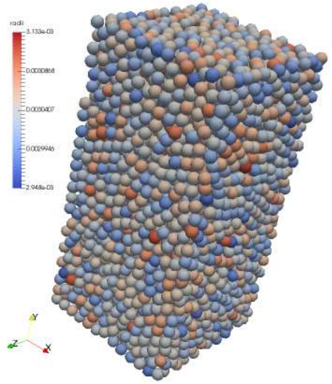
Porous Media Model

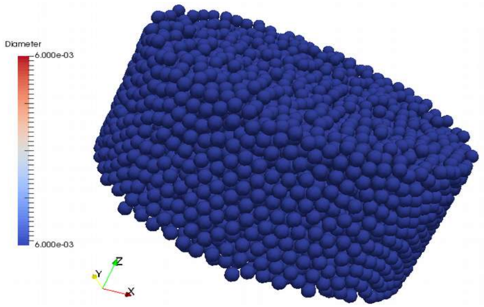
CFD (FVM)

FLUENT

OpenFOAM

Other possibilities of investigations

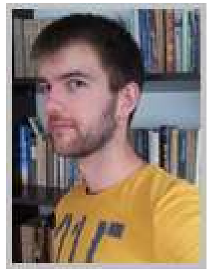


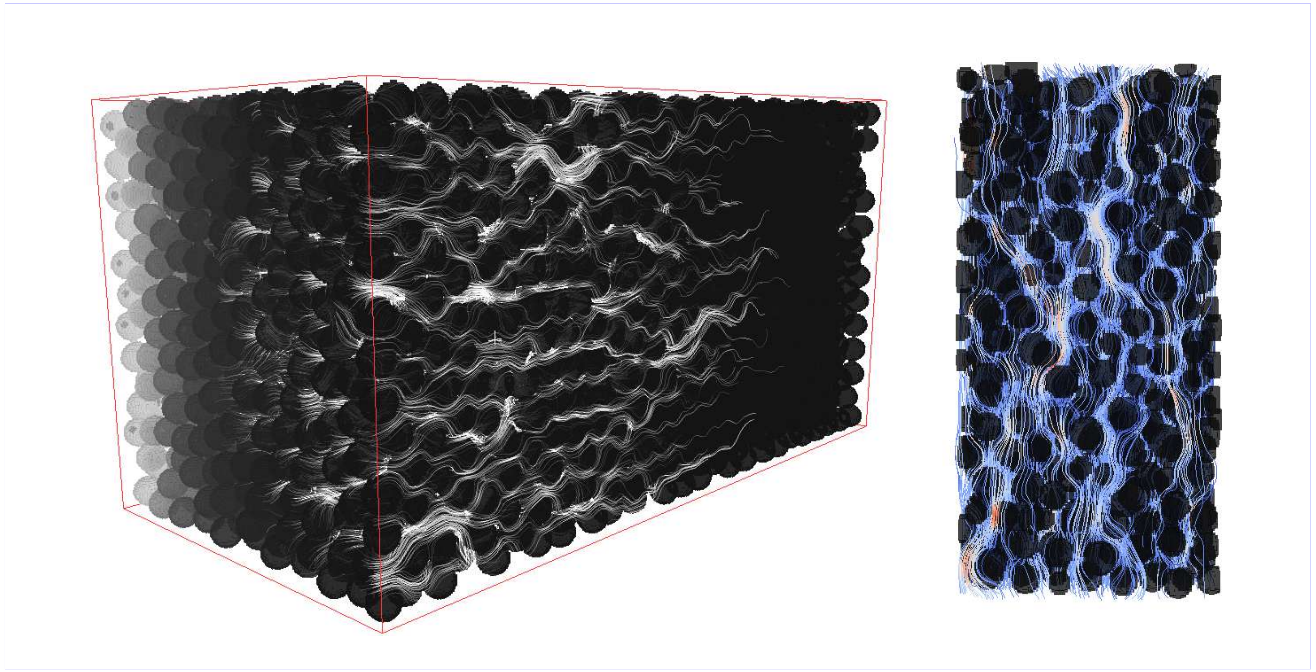


$$n_i, x_i, y_i, z_i, d_i$$

Maciej Matyka

Jarosław Gołembiewski





Linking with the Lattice Boltzmann Method (Palabos)

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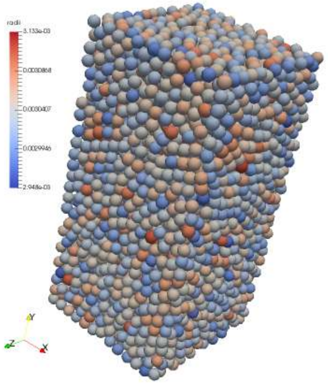
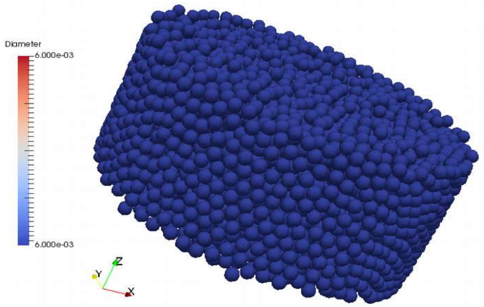
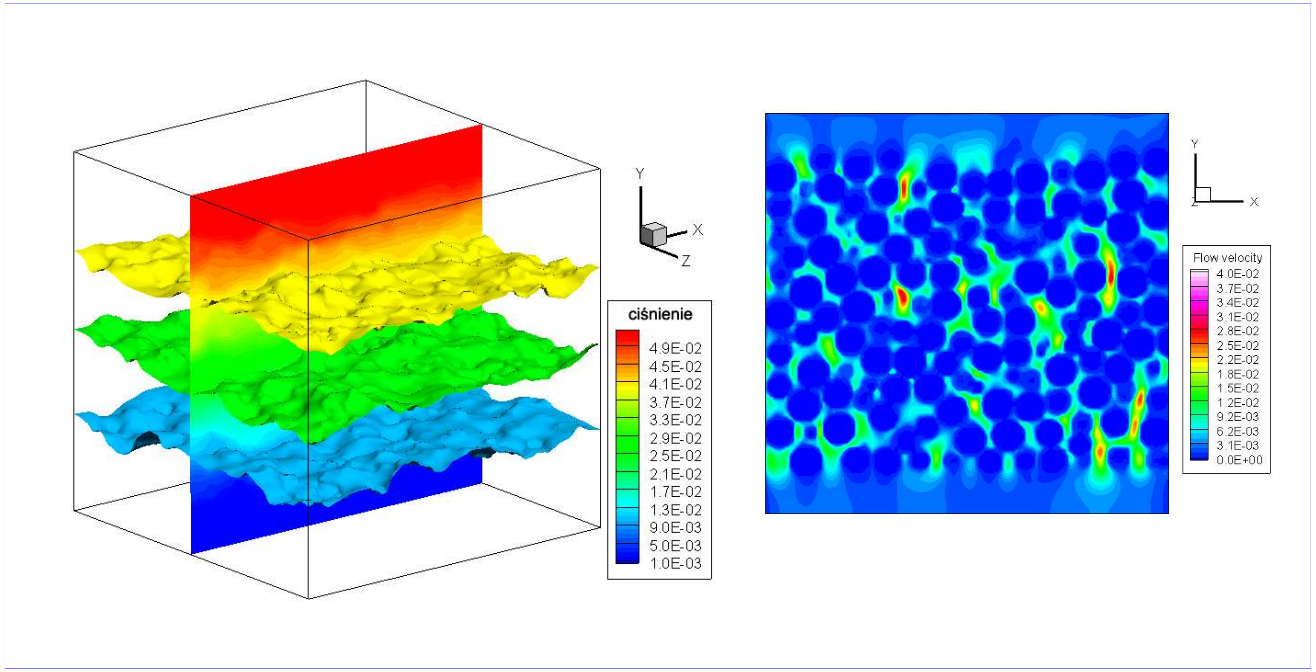
Other possibilities of investigations



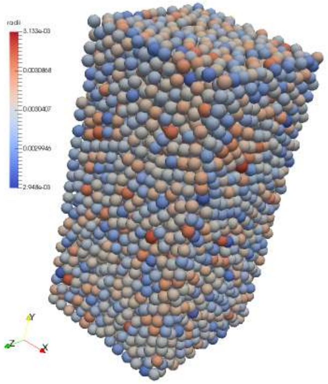


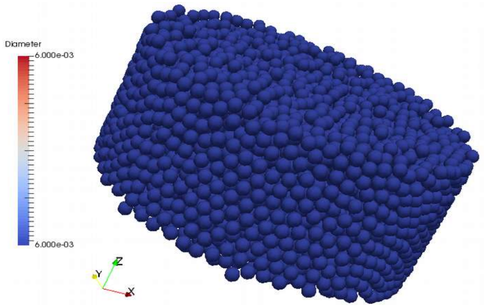
$$n_i, x_i, y_i, z_i, d_i$$

Maciej Marek



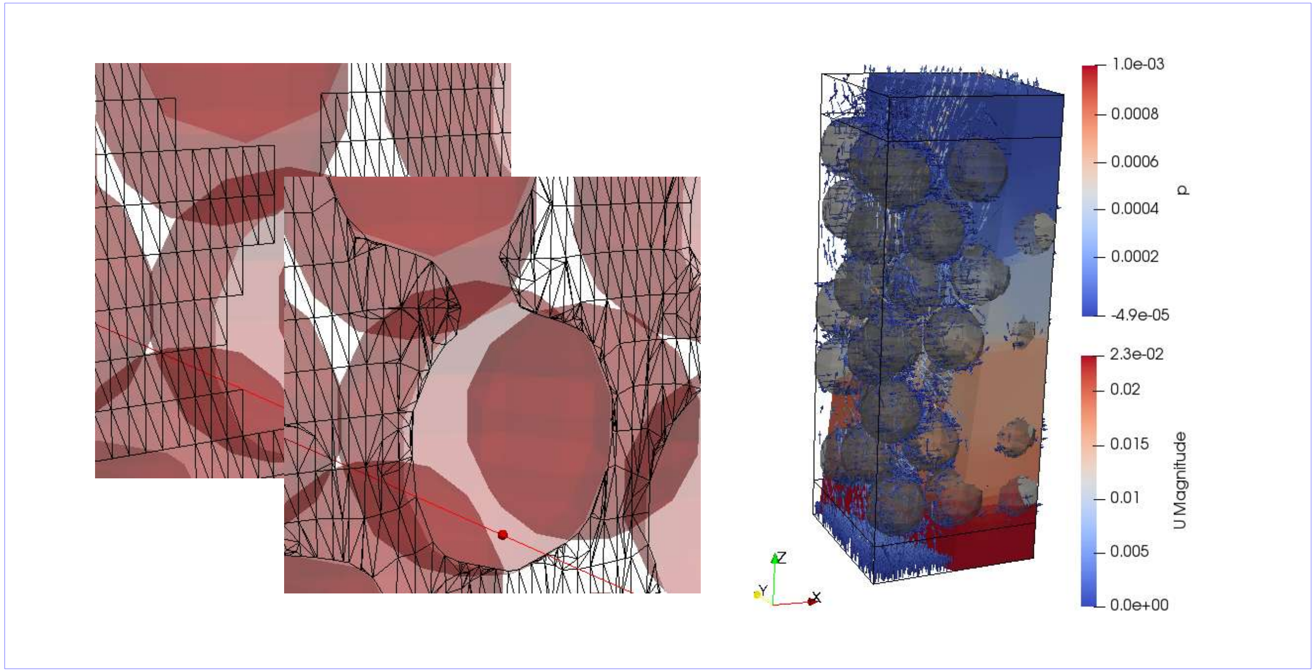
Linking with the
Immersed Boundary Method
(code written by M. Marek)





Other possibilities of investigations

$$n_i, x_i, y_i, z_i, d_i$$



Linking with the
Finite Volume Method
(OpenFOAM)

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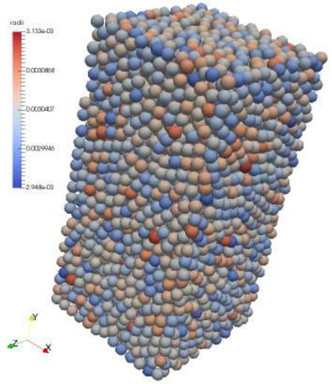
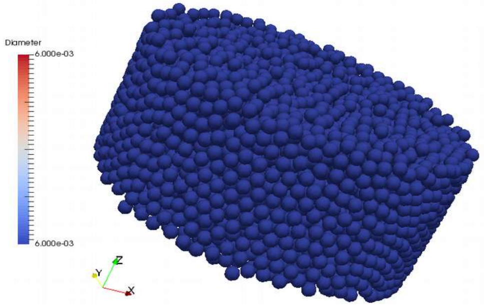
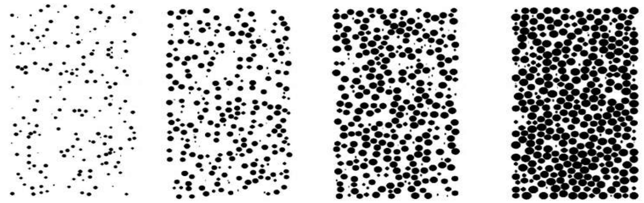


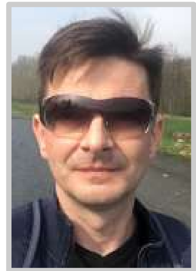


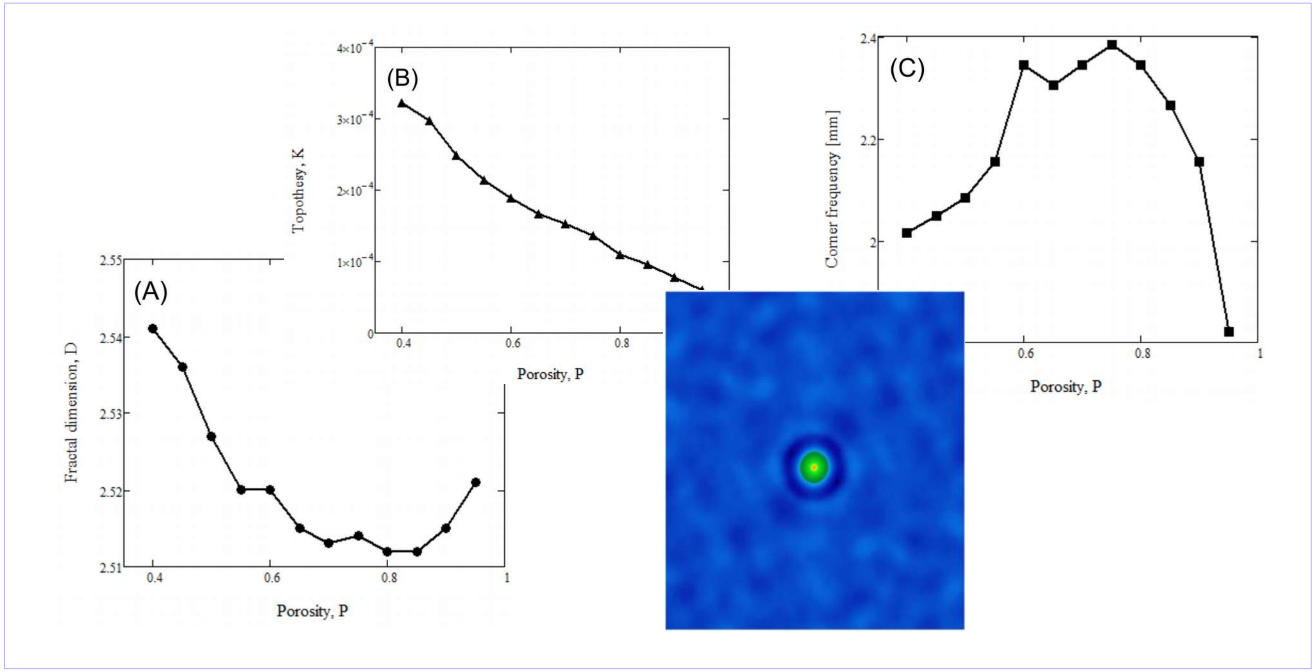
Other possibilities of investigations



$$n_i, x_i, y_i, z_i, d_i$$

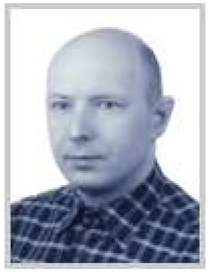
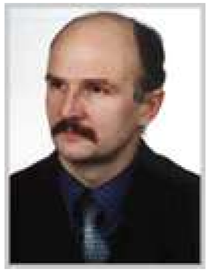
Mirosław
Bramowicz

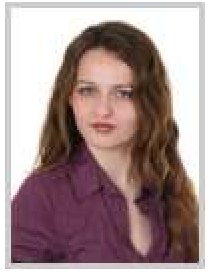


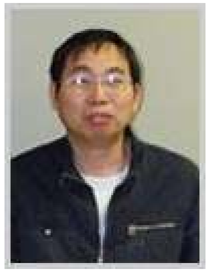


Linking with
methods of fractal analysis
(code written by M. Bramowicz)




Cooperation in the framework
of the PathFinder Project:
http://www.uwm.edu.pl/pathfinder/

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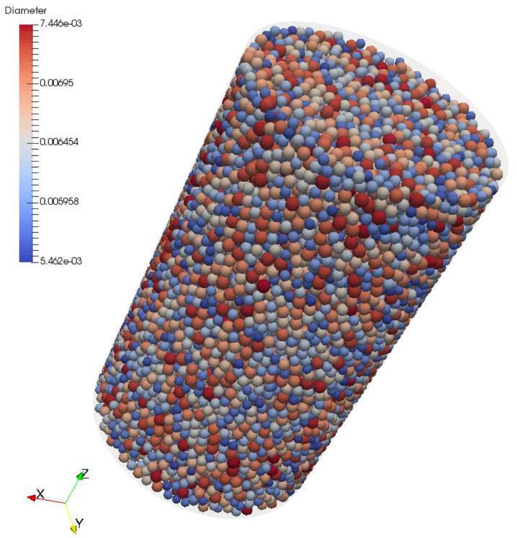

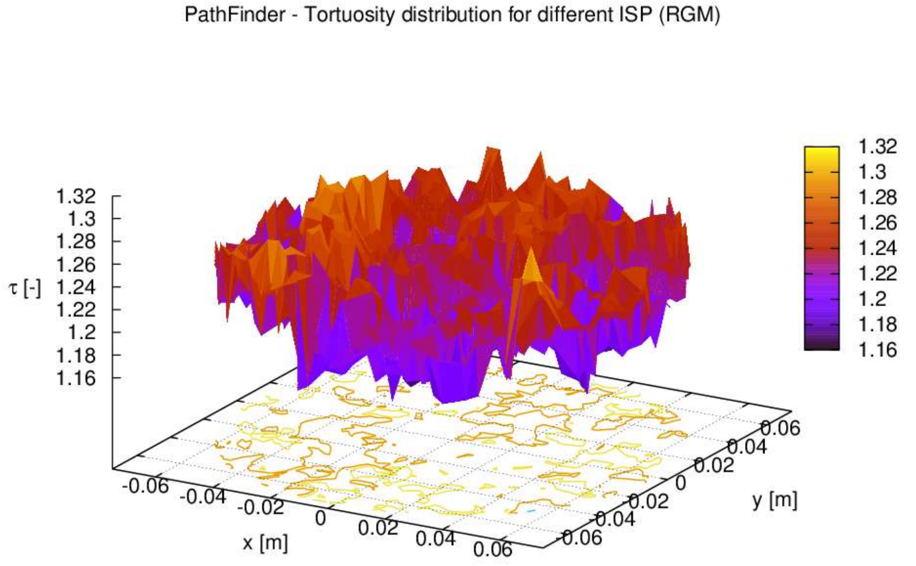

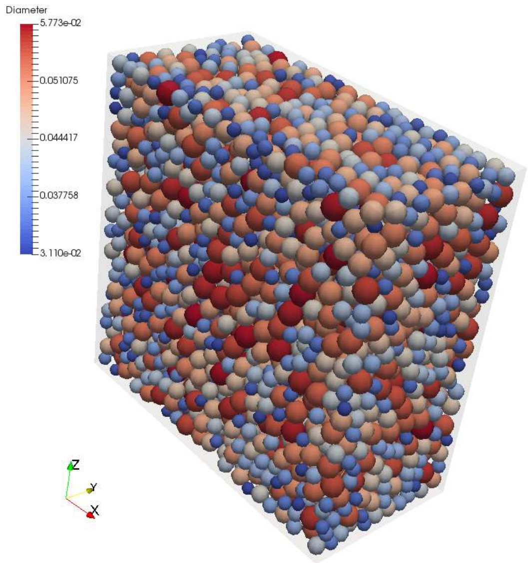

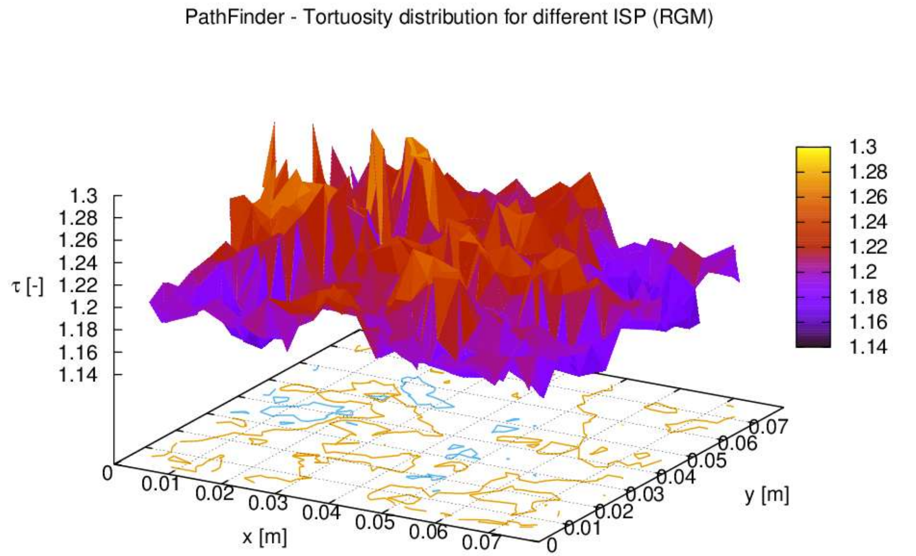

Examples of own investigations: determination the tortuosity fields in the dominant flow direction (with the use of the Regular Grid Method)

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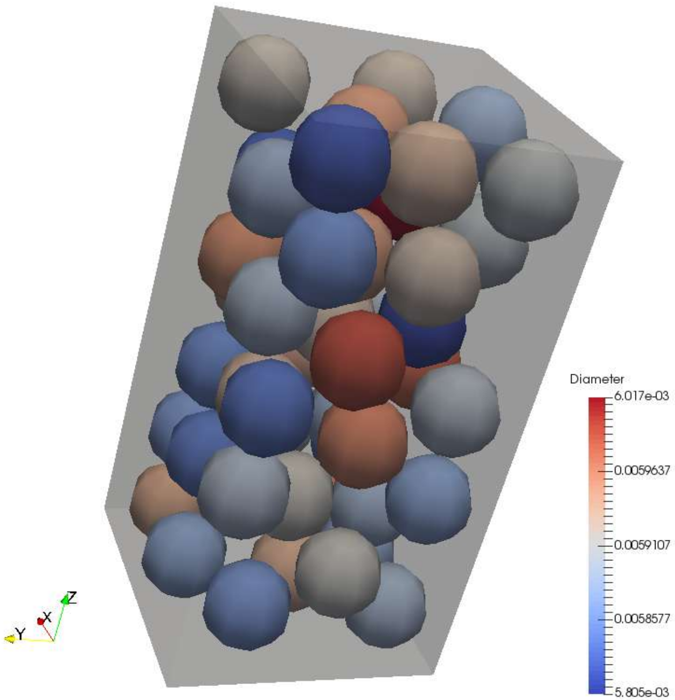
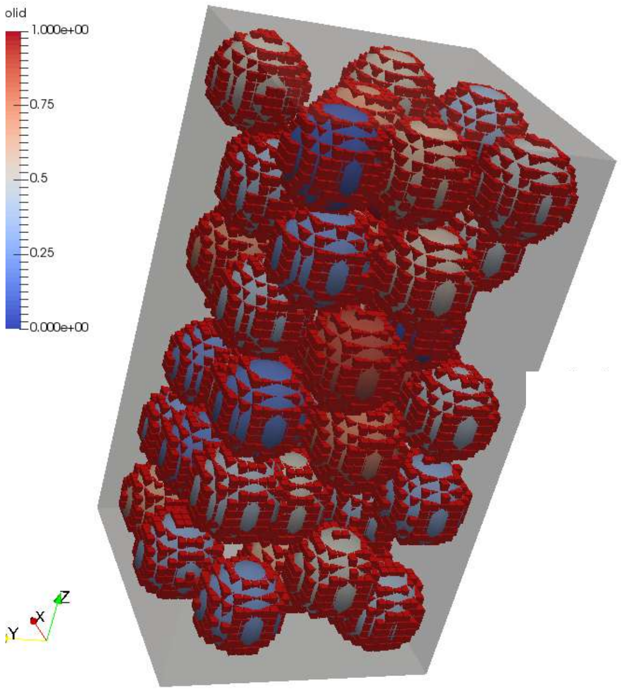
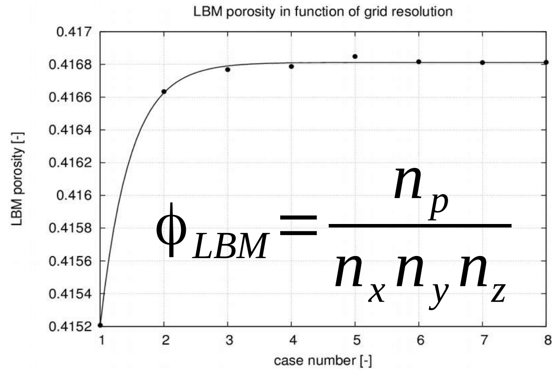


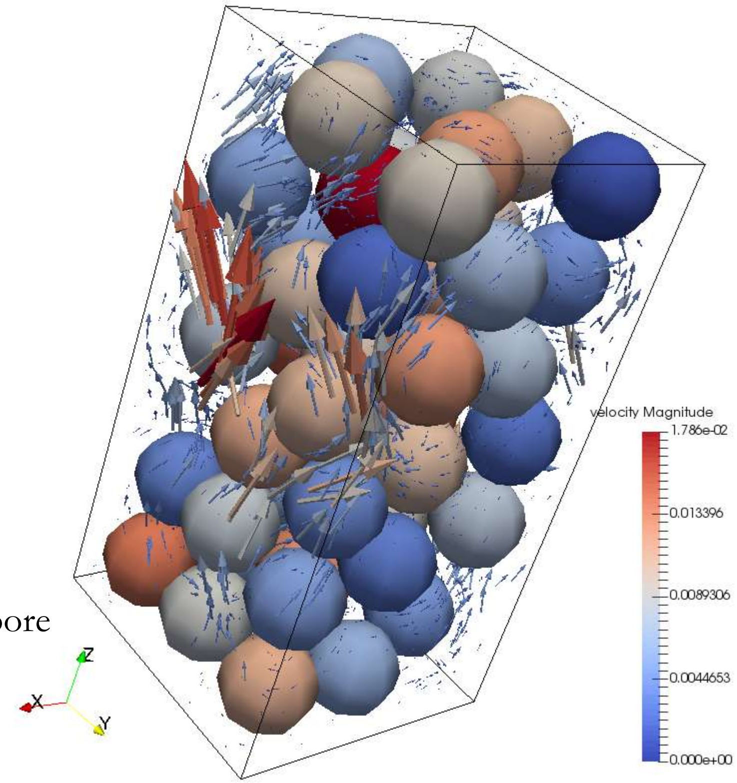
Virtual bed (YADE)



Conversion to the lattice geometry (own code)



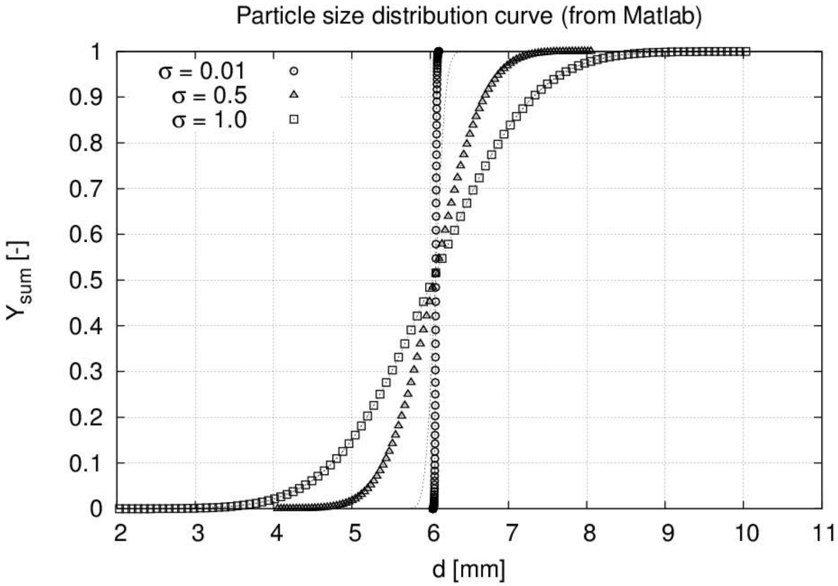
$$\phi_{LBM} = \frac{n_p}{n_x n_y n_z}$$



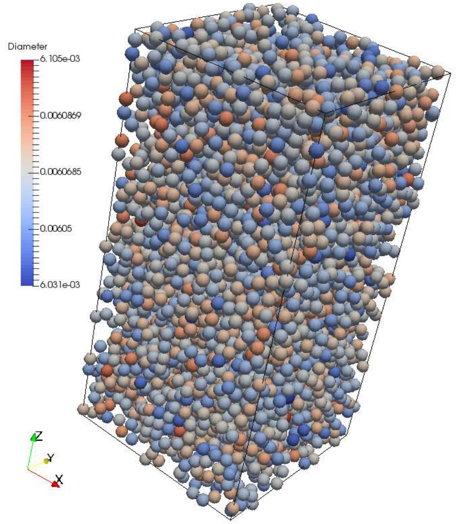
Velocity field in the pore space (Palabos)

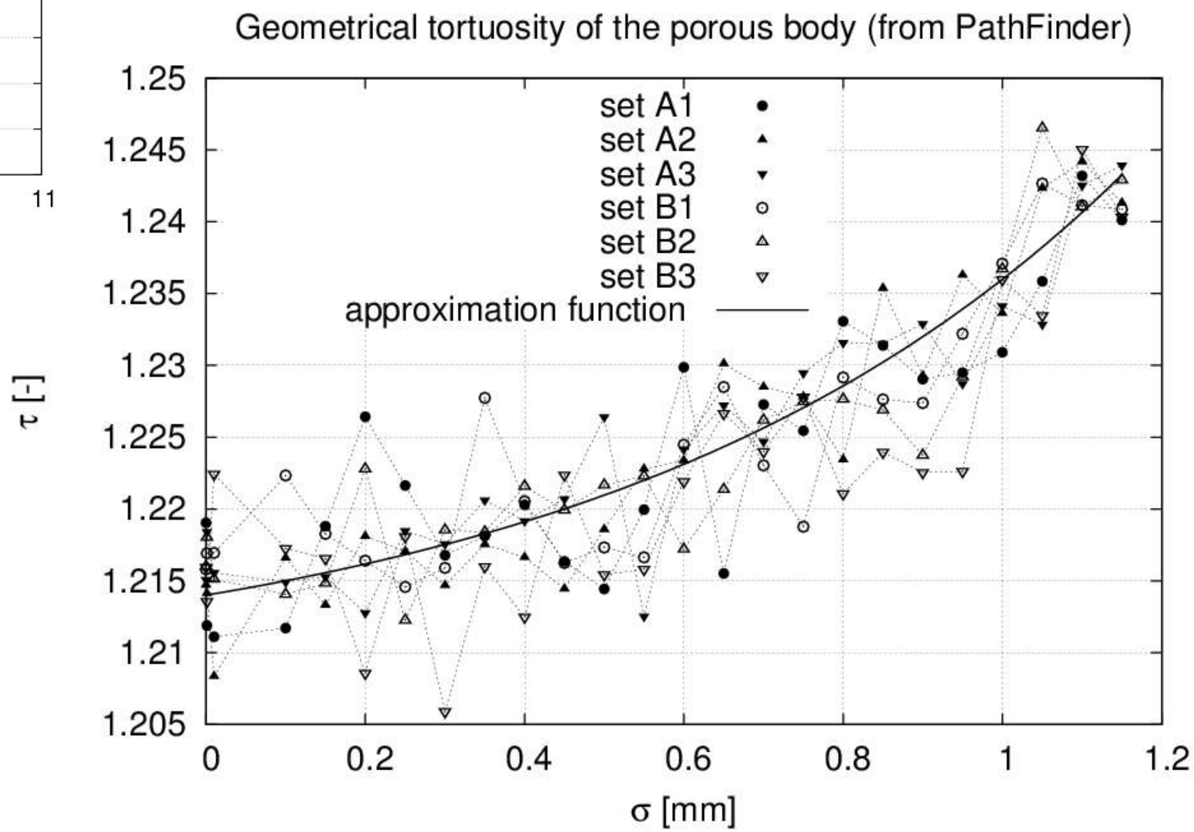
Examples of own investigations: applying the Lattice Boltzmann Method for modeling the fluid flow through the pore space

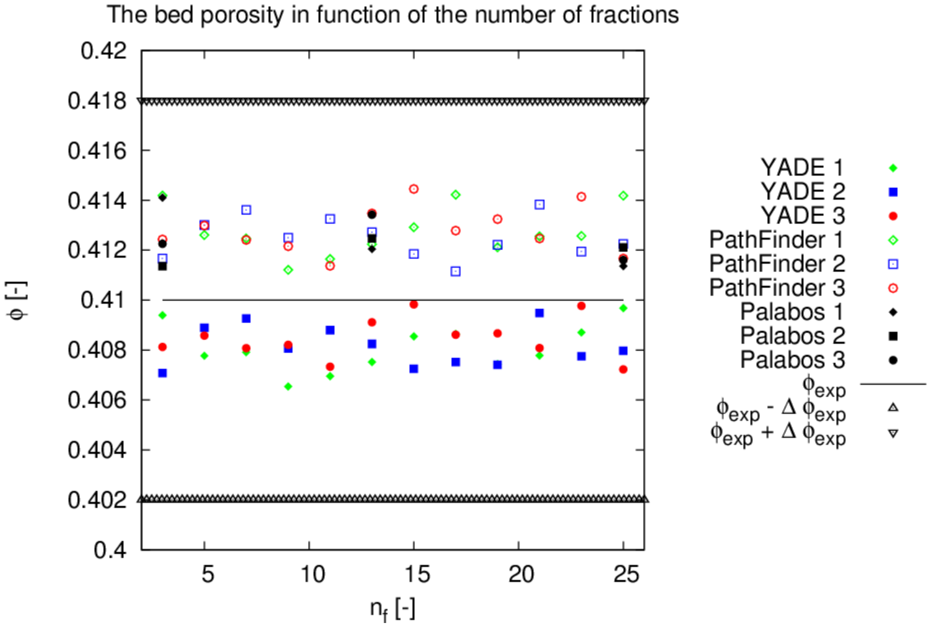
Sobieski W.: http://pracownicy.uwm.edu.pl/wojsob/ (in Polish)

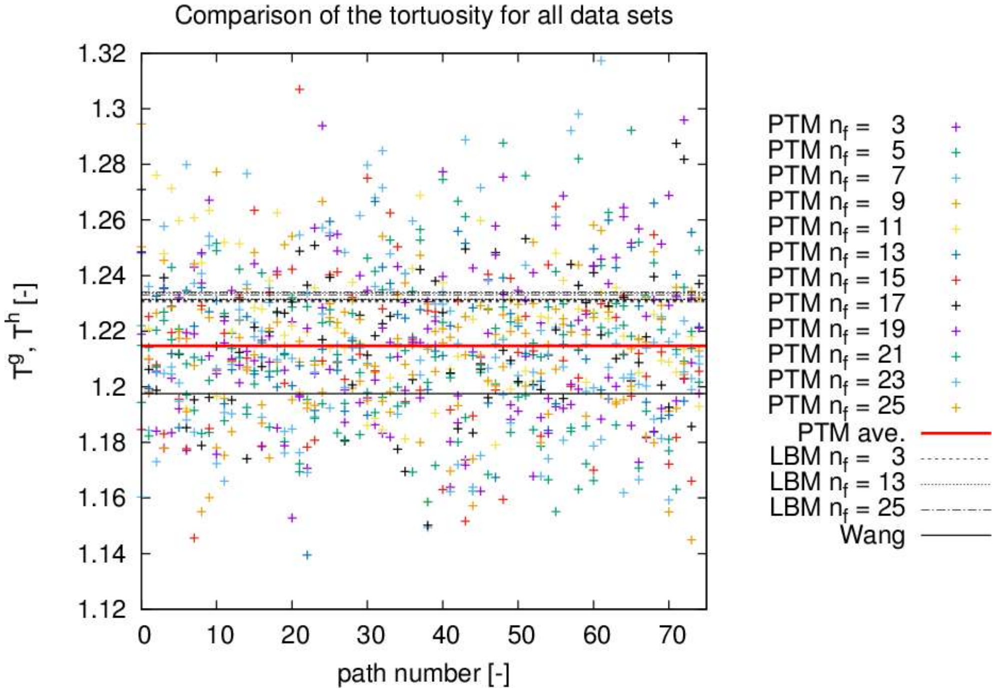


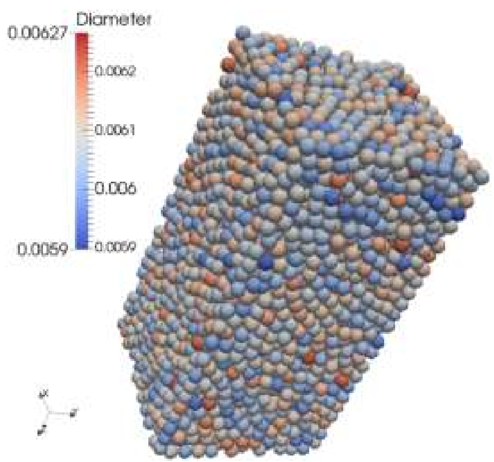
Examples of own investigations (in cooperation with S. Lipiński): study of the influence of particle distribution on the elements of the set Φ

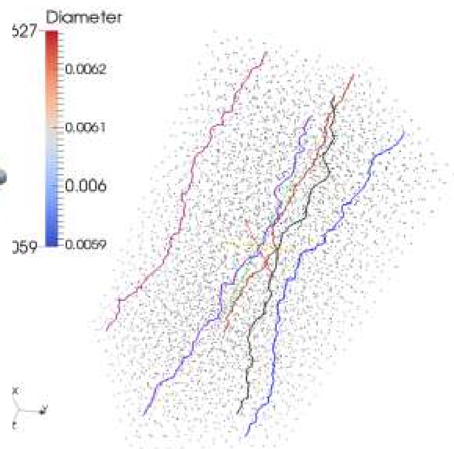












Examples of own investigations (in cooperation with M. Matyka, J. Gołembiewski and S. Lipiński: comparison of geometric tortuosity (PathFinder) and hydraulic tortuosity (LBM, Palabos)

- **Sobieski** W.: Numerical investigations of tortuosity in randomly generated pore structures. MATHEMATICS AND COMPUTERS IN SIMULATION (2019) DOI: https://doi.org/10.1016/j.matcom.2019.04.005.
- **Sobieski** W., Matyka M., Gołembiewski J., Lipiński S.: The Path Tracking Method as an alternative for tortuosity determination in granular beds. GRANULAR MATTER, Vol. 20:72 (2018), 14 p.
- Bramowicz M., Kulesza S., **Sobieski** W.: Characteristics of porous beds based on fractal parameters. TECHNICAL SCIENCES, Vol. 20, No 2 (2017).
- **Sobieski** W., Lipiński S.: The analysis of the relation between porosity and tortuosity in granular beds. TECHNICAL SCIENCES, Vol. 20, No 1 (2017), pp. 75-85.
- **Sobieski** W., Lipiński S., Dudda W., Trykozko A., Marek M., Wiącek J., Matyka M., Gołembiewski J.: "Granular porous media" [monograph] (in Polish). Department of Mechanics and Machine Design, Olsztyn 2016. ISBN 978-83-60493-04-5.
- **Sobieski** W., Zhang Q.: Multi-scale modeling of flow resistance in granular porous media. MATHEMATICS AND COMPUTERS IN SIMULATION, Vol. 132 (2017), pp. 159-171.
- **Sobieski** W., Dudda W., Lipiński S.: A new approach for obtaining the geometric properties of a granular porous bed based on DEM simulations. TECHNICAL SCIENCES, Vol. 19, No 2 (2016), pp. 165-187.
- **Sobieski**, W.: The use of Path Tracking Method for determining the tortuosity field in a porous bed. GRANULAR MATTER (2016) 18:72. DOI:10.1007/s10035-016-0668-3.
- **Sobieski** W., Trykozko A.: Darcy's and Forchheimer's laws in practice: Part 2. The numerical model. TECHNICAL SCIENCES, Vol. 17, No. 4 (2014), pp. 337-350.
- **Sobieski** W., Trykozko A.: Darcy's and Forchheimer's laws in practice: Part 1. The experiment. TECHNICAL SCIENCES, Vol. 17, No. 4 (2014), pp. 321-335.
- **Sobieski** W., Zhang Q.: Sensitivity analysis of Kozeny-Karman and Ergun equations. TECHNICAL SCIENCES, Vol. 17, No. 3 (2014), pp. 235-248.
- Dudda W., **Sobieski** W.: Modification of the PathFinder algorithm for calculating granular beds with various particle size distributions. TECHNICAL SCIENCES, Vol. 17, No 2 (2014), pp. 135-148.
- **Sobieski** W., Zhang Q., Liu, C.: Predicting tortuosity for airflow through porous beds consisting of randomly packed spherical particles. TRANSPORT IN POROUS MEDIA, Vol. 93. No. 3 (2012), pp. 431-451. DOI: 10.1007/s11242-012-9961-8.
- **Sobieski** W.: Calculating tortuosity in a porous bed consisting of spherical particles with known sizes and distribution in space. Research report 1/2009, Winnipeg (Canada), 2009.

Thank you for watching