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Jean-Yves Delenne, Vincent Richefeu, Xavier Frank, Farhang Radjai

► **To cite this version:**

| Jean-Yves Delenne, Vincent Richefeu, Xavier Frank, Farhang Radjai. Flowbox. 2015. hal-01603489

HAL Id: hal-01603489

<https://hal.science/hal-01603489>

Submitted on 5 Jun 2020

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FLOWbox – User Guide

Jean-Yves Delenne

UMR IATE,
CIRAD, INRA, Montpellier SupAgro, Université de Montpellier,
F-34060 Montpellier, France

Vincent Richefeu

UMR 3SR,
Université Grenoble Alpes, 3SR, F-38000 Grenoble, France

Xavier Frank

UMR IATE,
CIRAD, INRA, Montpellier SupAgro, Université de Montpellier,
F-34060 Montpellier, France

Farhang Radjai

UMR LMGC,
Université de Montpellier - CNRS, F-34090 Montpellier, France

Abstract

This document describes how to use the code **FLOWbox** dedicated to the computation of flow through porous and granular materials. **FLOWbox** is based on an optimized 3D Lattice Boltzmann algorithm for the computation of liquid or gas flows directly at the scale of heterogeneities. **FLOWbox** intends to be a powerful and versatile software able to operate on highly detailed microstructures in a systematic fashion. These microstructures can be generated either from numerical simulation or from tomography.

Contents

1	Introduction	2
2	Basics of the Lattice Boltzmann Method	3
3	Running FLOWbox	4
4	Simulation file	5
4.1	Main command keywords	5
4.2	Sample file format	6
4.3	Output files	7
4.4	Parallel computing	8
5	Examples of simulations and graphical outputs	8
5.1	Flow around a sphere	8
5.2	Tomography picture	9
5.3	Packing	12

1 Introduction

FLOWbox is a Computational Fluid Dynamics (CFD) software based on the Lattice Boltzmann Method (LBM). A major advantage of the LBM over other computational fluid dynamics models is its high flexibility for the implementation of geometrically complex boundary conditions. FLOWbox compute the flow through 3D microstructures meshed using a rectilinear grid. These microstructures are composed of binary voxels (3D pixels) that can be generated from segmented pictures or tomography or rasterized 3D objects from Discrete Element Method (DEM) or Monte Carlo (MC) simulations.

FLOWbox main powerful features are:

- Computation of the fluid dynamics at the scale of the microstructure for sufficiently small Reynolds numbers. Detailed information such as velocities at the nodes, streamlines, vorticity, pressure gradients are easily assessable via a vtk interpreter such as Paraview (see www.vtk.org).
- Determination of pressure drop along the sample.
- Groups of voxels can be defined to integrate hydrodynamic forces on specific objects.
- FLOWbox implement bi-periodic boundaries to reduce finite size effects in the vicinity of the boundaries transverse to the direction of the flow.
- The command-line interface of FLOWbox is flexible, takes few of the computer resources, is easy to automate via scripting and thus is capable of massive run for extensive parametric studies¹. Although FLOWbox is better suitable to Unix-like operating systems, it can also run on MacOS or Microsoft Windows.

In the following we first recall the basics of the LBM, for developers we detail how to compile the sources and to generate the technical documentation. The control parameters are then specified together with the syntax of the simulation file and the 3D sample format. Finally we give some examples of feasible analysis using FLOWbox .

Notations used

The document uses the conventions listed below:

- `text that appear on the screen (Tele Type)`
- key
- *file_name*
- text of the document (Times)
- $\langle \text{var} \rangle$: variable (to replace by a value)
- [opt] : optional information
- Symbol \$: prompt

¹ Note that for this reasons, FLOWbox is not designed to embed a Graphic User Interface (GUI) which would have little practical interest.

2 Basics of the Lattice Boltzmann Method

The LBM is based on a material representation of fluids as consisting of particles moving and colliding on a lattice [2, 4, 5, 12]. Partial distribution functions $f_i(\vec{r}, t)$ are introduced to represent the probability density of a particle at the position \vec{r} at time t with a velocity $\vec{v} = \vec{c}_i$ along discrete direction i . `FLOWbox` uses D3Q19 meshing scheme, corresponding to 18 space directions in 3D. The distribution functions evolve at each node according to a set of rules, which are constructed so as to ensure the conservation equations of mass, momentum and energy, and thus to recover the incompressible Navier-Stokes equations [7]. This holds only when the wave lengths are small compared to the lattice spacing unit [3].

At each node, the fluid density ρ and velocity \vec{u} are defined as

$$\rho = \sum_i f_i. \quad (1)$$

$$\rho \vec{u} = \sum_i f_i \vec{c}_i. \quad (2)$$

and the temperature is given by

$$\frac{D}{2} kT = \sum_i \frac{1}{2} m (\vec{c}_i - \vec{u})^2 \frac{f_i}{\rho} \quad (3)$$

where m is particle mass and k is the Boltzmann constant. The equilibrium state is assumed to be governed by the Maxwell distribution:

$$f^{eq}(\vec{c}) = \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{m}{2kT} (\vec{c} - \vec{u})^2 \right) \quad (4)$$

where \vec{u} is the mean velocity. By expanding (4) to order 2 as a function of u/c_s , which is the local Mach number with c_s being the sound velocity, a discretized form of the Maxwell distribution is obtained and used in the LBM:

$$f^{eq} = \rho w_i \left(1 + b \frac{\vec{c}_i \cdot \vec{u}}{c_s^2} + e \frac{u^2}{c_s^2} + h \frac{(\vec{c}_i \cdot \vec{u})^2}{c_s^4} \right) \quad (5)$$

where the factor w_i and the coefficients b , e and h depend on the scheme with the requirement of rotational invariance [10]. The sound speed is then given by $c_s = \sum_i w_i c_i^2$. For the D3Q19 scheme, we have $c_s = c/\sqrt{3}$, where $c = \delta x / \delta t$ is the lattice velocity defined as the ratio of the basic lattice spacing δx to the LBM time step δt , and $c_s^2 = RT$. In LBM code unidimensionnal units called lattice units (lu) are commonly used and it is usual to set $\delta x = 1$, $\delta t = 1$ and $\rho = 1$ at equilibrium.

The velocities evolve according to the Boltzmann equation. In its discretized form, it requires an explicit expression of the collision term. We used the Bhatnagar-Gross-Krook (BGK) model in which the collision term for each direction i is simply proportional to the distance from the Maxwell distribution [1]:

$$\frac{\partial f_i}{\partial t}_{coll} = \frac{1}{\tau} (f_i^{eq}(\vec{r}, t) - f_i(\vec{r}, t)) \quad (6)$$

where τ is a characteristic time. Hence, for the D3Q19 scheme, we have a system of 18 discrete equations governing the distribution functions:

$$f_i(\vec{r} + \vec{c}_i \delta t, t + \delta t) = f_i(\vec{r}, t) + \frac{1}{\tau} (f_i^{eq}(\vec{x}, t) - f_i(\vec{r}, t)) \quad (7)$$

Physical parameters	Relationship with unidimensionnal parameters
Density	$\rho_0 \rho$
Kinematic viscosity	$c_s \delta x \nu$
Spatial coordinates	$\delta x \vec{x}$
Velocities	$c_s \vec{v}$
Acceleration	$\frac{c_s}{\delta t} \vec{a}$
Hydrodynamic forces	$\rho_0 c_s^2 \delta x \vec{F}$

Table 1: Relationship between physical parameters and unidimensionnal LBM parameters

These equations are solved in two steps. In the collision step, the variations of the distribution functions are calculated from the collisions:

$$\tilde{f}_i(\vec{r}, t + \delta t) = f_i(\vec{r}, t) + \frac{1}{\tau} (f_i^{eq}(\vec{r}, t) - f_i(\vec{r}, t)) \quad (8)$$

where the functions \tilde{f}_i design the post-collision functions. In the streaming step, the new distributions are advected in the directions of their propagation velocities:

$$f_i(\vec{x} + \vec{c}_i \delta t, t + \delta t) = \tilde{f}_i(\vec{x}, t + \delta t) \quad (9)$$

The above equations are supplemented by an equation of state, which is obtained by identifying the Navier-Stokes equations with the above equations [3]:

$$P(\rho) = \frac{1}{3} \rho \quad (10)$$

with kinematic viscosity given by

$$\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right) \quad (11)$$

and $\tau > 1/2$.

A major advantage of the LBM over other computational fluid dynamics models is its high flexibility for the implementation of geometrically complex boundary conditions. For example, the no-slip boundary condition at a wall or at the surface of an object immersed in the fluid simply implies zero velocity at the nodes belonging to the wall surface. This condition can be imposed by requiring that the fluid particles bounce back at the nodes. The fluid forces on the particles are calculated from the balance of momenta at the nodes belonging to the interface [2, 8, 9, 11].

Finally, note that it is possible to convert the parameters determined in LBM units to physical units using the relationships given in Table 1.

3 Running FLOWbox

To run a simulation with FLOWbox type in a terminal the following commands:

```
$ flowbox my_parameters.sim
```

Here, we assume that the application `flowbox` is in a path known by the system and that the file `my_parameters.sim` is in the current path. If not, you must specify the complete path. For instance:

```
$ ~/bin/flowbox my_parameters.sim
```

Note that if the source code of FLOWbox needs to be compiled you may type from a terminal prompt:

```
$ cd flowbox
$ make
```

The software command line utility *flowbox* will be created in the current directory.

4 Simulation file

A simulation file is a text file containing all the data and commands required to perform the computation. An example of this file is given in 1. We commonly use the *.sim* extension but FLOWbox can open every text file assuming the keywords commands are called with convenient values of parameters. Note that it is possible add to comment to this file using *!* or *#* at the beginning of the line.

```
! Example of command file
! result_folder ./RESULTS
vtkPeriod 100
pressureProfilePeriod 100
flowPeriod 2
num_threads 8

sample sample.txt
lzInf 15
lzSup 20

tau 0.6

rho_inlet 1.001
rho_outlet 1.0

step 0
step_max 100000000000
```

Code 1: Example of simulation file.

4.1 Main command keywords

In this section we list the most usual keywords commands usable in the command file. Note that there is no need to use them in a specific order but their syntax and number of arguments should be strictly respected.

vtkPeriod (integer)**period**

Set the number of steps to be done between two vtk files.

vtrPeriod (integer)**period**

Set the number of steps to be done between two vtu files.

vtkPeriod (integer)**period**

Set the number of steps to be done between two tecplotPeriod files.

pressureProfilePeriod (integer)**period**

Set the output period of the average pressure profile across the sample.

<code>flowPeriod</code>	(integer) <code>period</code>	Set the output frequency of inflow and outflow into the <i>flow.txt</i> file.
<code>num_threads</code>	(integer) <code>number</code>	Set the number of cores used in parallel computation.
<code>sample</code>	(string) <code>filename</code>	Set the sample file name. This file must be in the directory of FLOWbox
<code>lzInf</code>	(integer) <code>length</code>	Size in lattice units of the lower inlet. A layer of about 15 voxels is used to avoid strong pressure concentration at the boundary of the sample.
<code>lzSup</code>	(integer) <code>length</code>	Idem but for the upper bound at the outlet.
<code>tau</code>	(double) <code>characteristic time</code>	$\langle \tau \rangle$ or τ is a critical parameter that control the fluid viscosity in LBM simulation.
<code>rho_inlet</code>	(double) <code>density</code>	The $\langle \text{rho_inlet} \rangle$ parameter control the applied pressure at the inlet of the flow domain via the equation of state 10. Note that the code compute the relative pressure $P(\rho) = \frac{1}{3}(\rho - \rho_0)$ instead of absolute pressure.
<code>rho_outlet</code>	(double) <code>density</code>	Idem for the outlet of the flow domain.
<code>step</code>	(integer) <code>time step</code>	First time step of the simulation.
<code>step_max</code>	(integer) <code>time step</code>	Last time step of the simulation.

4.2 Sample file format

A sample file may be used to define the microstructure of the sample from a tomographic images of simulation results. The file format is very simple. The sample code 4.2 illustrate the structure of the file for a squared pipe. The first 3 values gives the number of voxels along x , y and z axis. Then all the values are given by going through x first then y and finally z . The 0 values represent the fluid domain and the positive values are used to define solid zones into the sample. In the example file 4.2 the 1 values define the boundary of the pipe.

```

10 10 100
1 1 1 1 1 1 1 1 1 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 1 1 1 1 1 1 1 1 1

...

1 1 1 1 1 1 1 1 1 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 0 0 0 0 0 0 0 0 1
1 1 1 1 1 1 1 1 1 1

```

Code 2: Example of sample file structure.

4.3 Output files

When running FLOWbox different output files are created and putted by default in the **RESULT** folder.

There are basically three types of file:

- The **flow.txt** file gives the evolution of pressure at the inlet and outlet as a function of time.
- The **zpressXXX.txt** files, where **XXX** gives the number of the file². These files can be used to determine the pressure drop along *z* axis.
- The **resultXXX.vtk**, **resultXXX.vtr** or **resultXXX.dat** files store the fields data into the whole domaine. The first two file format **.vtk** and **.vtr** can be directly open using Paraview (www.paraview.org) and **.dat** files can be open using Tecplot (www.tecplot.com)³. In these files, the accessible data are the pressure and velocity field at each nodes and an identification parameter named **zone** used to specify whether the voxel is of solid or fluid type.

² It is possible to get the time step by multiplying this number by the **period** specified in the simulation file.

³ Note that Paraview is a free software.

Note that as `txt`, `vtk`, `dat` formats are written in ascii it is possible to directly read the data using a simple text editor. For example the `txt` results can be directly plotted using Microsoft Excel or Gnuplot. On the contrary `vtr` is a binary format that can be open only with specific softwares. The main interest of this format is that it uses much less memory than standard `vtk`.

4.4 Parallel computing

FLOWbox has parallel computing capabilities based on OpenMP standards. The number of threads may be set using `wanted_num_threads` in the configuration file. Even if important speedup may be achieved, the running time highly depends on available memory and on the CPU usage of the operating system and other softwares. Note that the CPU number of cores corresponds to the number of threads if no hyper-threading is activated so that the number `wanted_num_threads` should not be greater than two times the total number of cores.

5 Examples of simulations and graphical outputs

In this section we presents several examples of FLOWbox usage in order to highlight its basic features.

5.1 Flow around a sphere

FLOWbox implement a simple sphere geometry primitive useful for simple benchmark tests. In the example file 3 we set a fluid domain of 40 voxels and add a sphere of radius 8 voxels. The `place_sphere` command is used to setup the x , y , and z coordinates of the center of the sphere, the radius R and the sphere id⁴.

⁴ Note that this value should be greater or equal to 1

```

! Example of command file
! result_folder ./RESULTS
vtrPeriod 100
pressureProfilePeriod 100
flowPeriod 2
num_threads 8

lxSample 80
lySample 80
lzSample 80
resize
place_sphere 40 40 40 8 1
setSolidBounds

rho_moy      1.0

tau  0.6

rho_inlet  1.001
rho_outlet 1.0

step 0
step_max 1000000000000

```

Code 3: Example of command file source for computing the flow around a spherical particle.

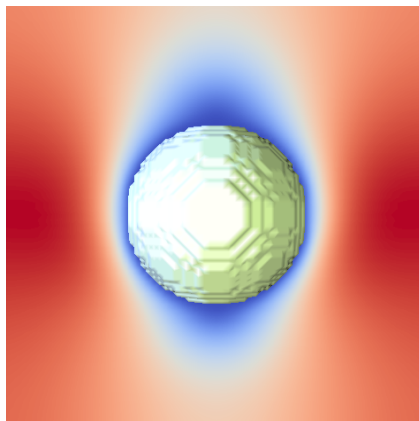


Figure 1: Example of velocity flow around a sphere.

Figure 1 shows an example plotted using Paraview of the velocity field around a spherical particle immersed in an horizontal flow.

5.2 Tomography picture

In this example we use a tomography picture of wood vessels (figure 2) from [6]. To avoid singularities at the boundary we added 15 voxels at the inlet and outlet using `lzInf 15` and `lzSup 15` commands in the simulation file.

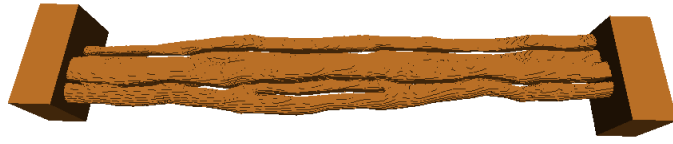


Figure 2: Tomography of wood vessels [6]. Note the two reservoir used to homogenize the pressure at the inlet and outlet of the domain.

Figure 3a and 3b show the pressure gradient and displays several stream lines in the sample.

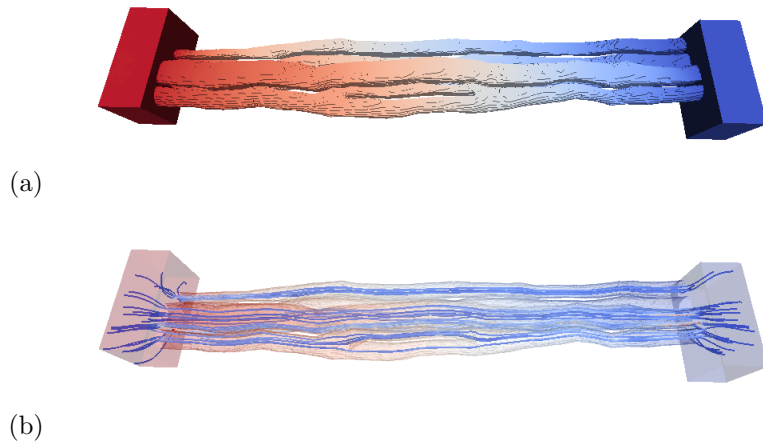


Figure 3: Flow through wood vessels: (a) Pressure gradient; (b) Stream lines

Figures 5.2a and 5.2b display velocity profiles in several cross sections perpendicular to the flow direction.

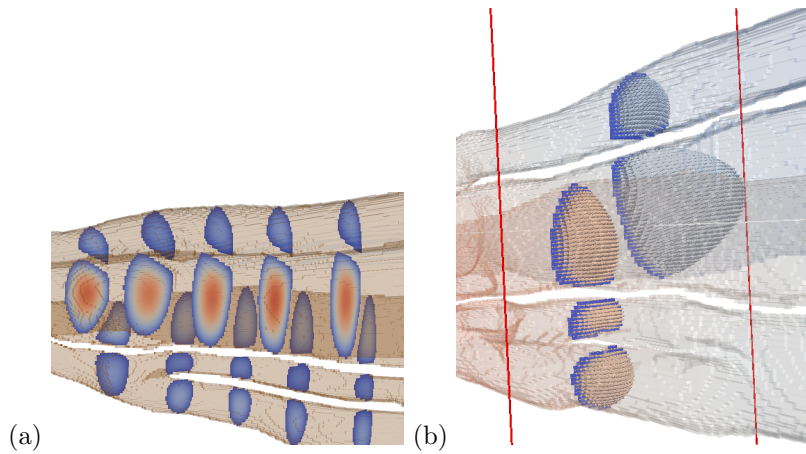


Figure 4: (a) magnitude of velocity field (in color map) at different position in the sample. (b) Velocity in a slice plotted using glyph vectors.

In figure 5 we plotted in semi-log axis the ratio of P_{in} and P_{out} as a function of time (in lattice units). After a rapid fluctuating domain the flow becomes stationary.

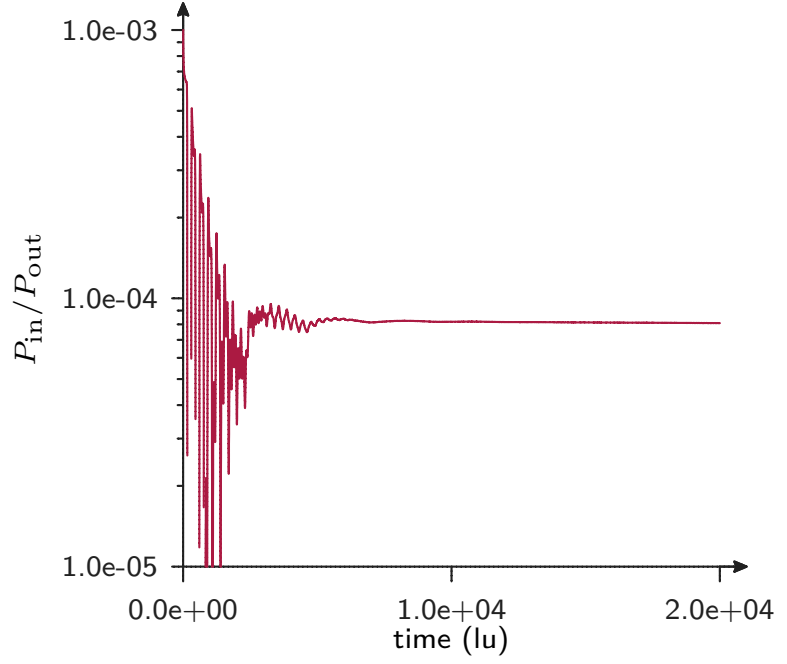


Figure 5: Evolution of P_{in}/P_{out} as a function of time.

In the stationary regime, we plot in figure 6 the average pressure evolution in z slices as a function of z/L_x . Where L_x is the size of the sample in x direction. This evolution is a straight line grow which it is possible to determine the permeability using the Darcy law.

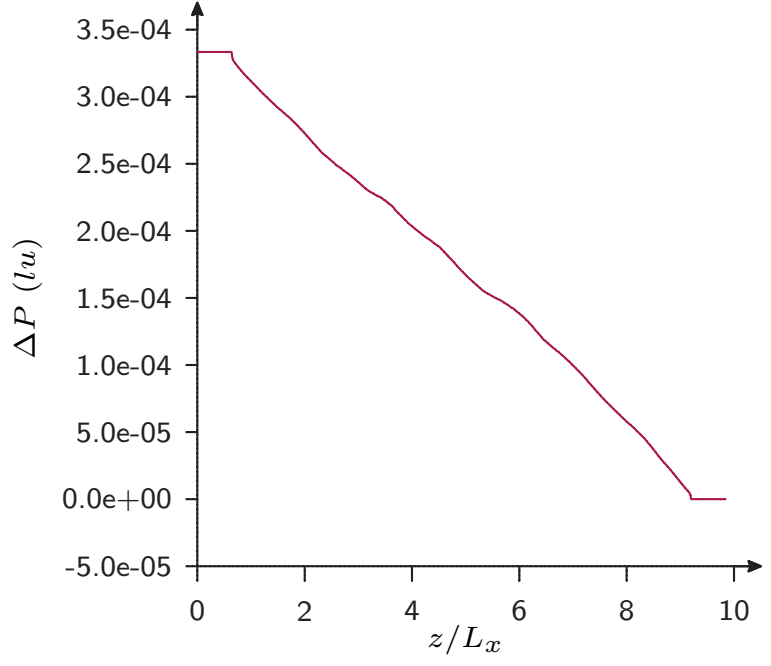


Figure 6:

5.3 Packing

In this section we give an example in which the samples has been compute form Monte Carlo simulations. This sample is composed of particles of different sizes packed together in a periodic cell. Figure 7a shows a magnified picture of the particles and figure 7b the sample rasterized sample used in FLOWbox .

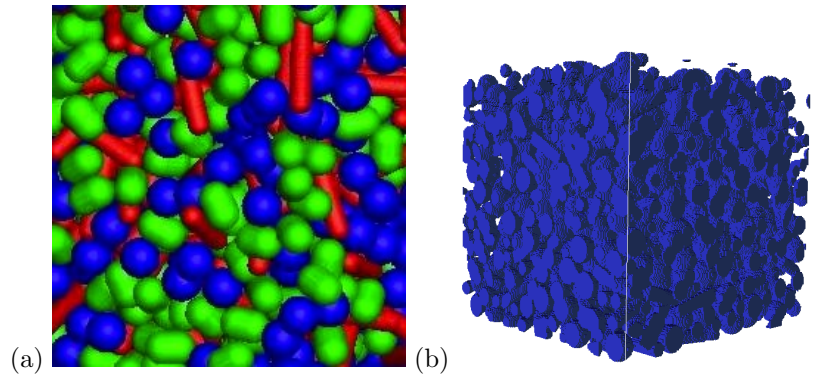


Figure 7: (a) Packing of particles; (b) Rasterized sample.

The figure 8 shows the pressure gradient and streamlines through the packing plotted using Tecplot.

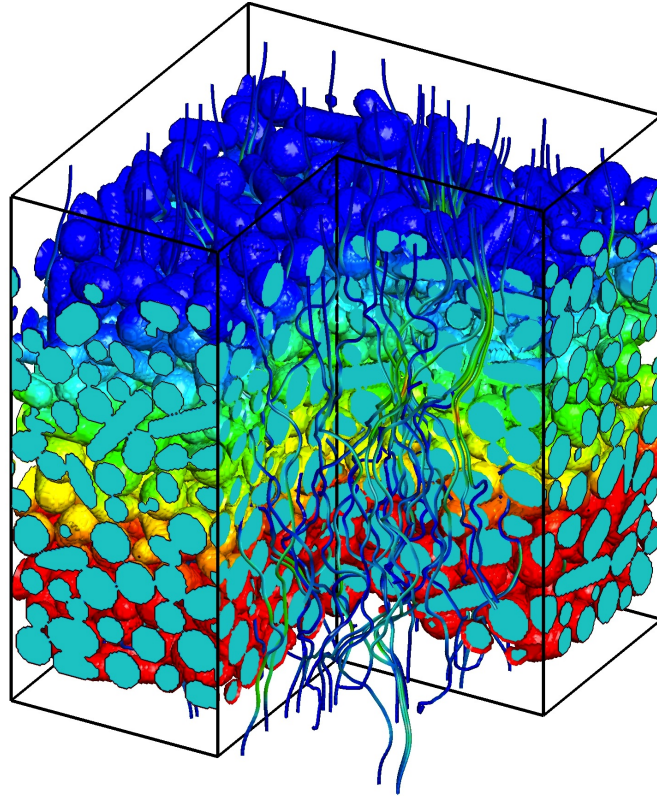


Figure 8: Flow through a sample of spherocylindrical particles of different length.

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