COMPUTER SIMULATION AND MODELING OF LIQUID DROPLETS DEPOSITION ON NANOFIBRES

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Abstract
The research team deal with computer simulation, procedural modeling, and visualization of stereometric liguid transport in fibrous materials. In this report there is used discrete model based on the idea of 3-D Ising model. After construction of statistical model, a couple of computer simulations, optimization of computed scientific data, there is need to visualize this one with possibility of feedback. It leads to apply open source software framework as visual instrument for this purposes where it is used like a visualizer of previously computed scientific data. Procedure is very simple otherwise efficient due to possibilities of modified oss application. After pretty much Monte-Carlo simulation steps are occupied elements of 3D model imported in layers into as vertices. Then is apply a volumetric effect on them (various color depending on fibre or liquid fluid element). Further is possible render or animate structures made by fibres with liquid interaction or even cut samples in desired positions with orthographic camera point of view. It works properly actually for very large data sets.
Key words: computer visualization, procedural modeling, nanoporous media, transport phenomena

Introduction

A flow involving more than a single phase is classified as multiphase or nonhomogeneous, such as liquid flows in porous fiber media, and we are interested in the dynamics of the evolving interface between the distinct phases during such nonhomogeneous flows in a fiber mass. The dynamics of such flow are dominated by surface tensions, porous media anisotropy and nonhomogenity, fiber volume fraction, and fiber wetting behaviors.

The uncertain structural conditions in fibrous media, including the susceptibility to even small loads, as well as the tortuous connectivity of their open pores and poorly defined boundaries, result in complex local nonhomogeneous flows and interfacial evolution. This complexity, in many cases, becomes prohibitive for the development of analytical theories describing these phenomena. The wetting and wicking of fiber mass constitute a class of flows that have critical scientific and first of all practical significance.

Idea

Adapt Monte-Carlo simulation based on the Ising model for a description of the wetting and wicking phenomena in fibrous media. We introduce here a 3-D Ising model, incorporated with the stochastic dynamics and the method of importance sampling, which enables us to interpret the model outputs in terms of wicking dynamics.

The essential principle of this model is based on the discretion of the whole system of a fibrous mass, a liquid source, and a wetting configuration at any given moment. The continuous media in the system, including the solid, liquid, and gas, are all divided as assemblies of individual cells occupied by the respective medium so that such a discrete system of cells can be manipulated more easily in a computer. The liquid wicking simulations are then set up from the initial configuration of the liquid layer into which the fiber mass with a predefined fiber orientation is in part vertically dipped, absorbing the liquid.

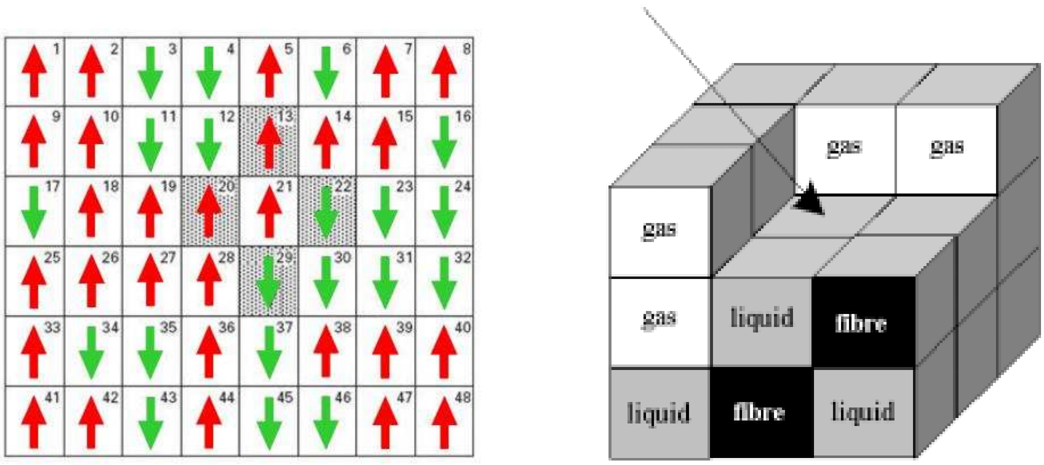

Figure 1. 2-D Ising basic ferromagnetic model vs 3-D Ising model for liquid-fiber mass interaction. A cell in the center to form a supercube with its neighboring cells. On the front surface, we can see various kinds of media that occupy the cells: the white color denotes the air, the grey color denotes the liquid, and fiber cells are black, for example.

Statistical physics in general deals with systems with many degrees of freedom. These degrees of freedom, in our case, are represented by the so called Ising variables. We assume that we know the Hamiltonian (the total internal energy) of the system. The problem is computing the average or equilibrium macroscopic parameters observable (energy and liquid mass uptake) for a given initial system configuration. Moreover, we will monitor the kinetics or even dynamics of the system so as to simulate the wicking behavior with time, see more [3],[4].

Model

The auto-model (particularly so called Ising model) and Monte-Carlo method were used especially for simulation of a liquid droplet in contact with fibrous material. Mechanism of this kind of simulation is fully described in [2].

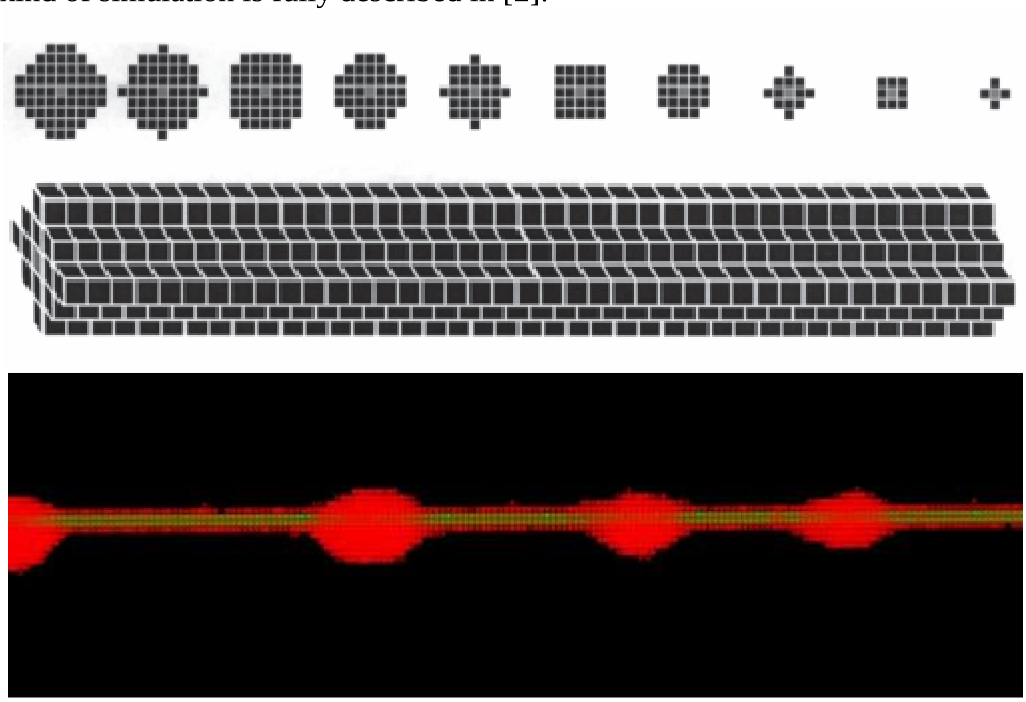

Figure 2. A simulation box with cells illustrate schematically 3-D Ising model of droplets on single fibre in various configurations. In this case for purpose of procedural modeling Rayleigh instability phenomena (top). Computer visualization of Rayleigh instability of liquid droplets on single fibre (down).

Methodology

With the use of an optimized algorithm, the 3-D Ising model improves accuracy and efficiency in simulation. This approach is capable of realistically simulating the complicated mechanisms involved in the filtration and separation processes. The fibrous material represented nonwoven material.

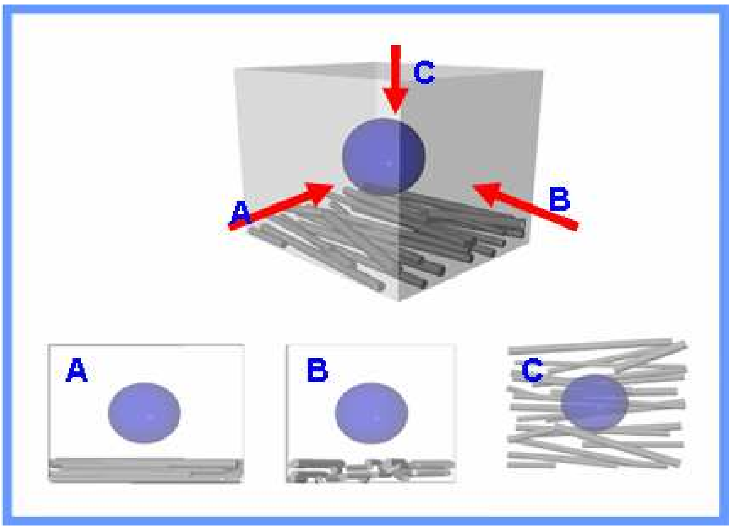

Figure 3. An illustration of initial state of simulated system. Dropping ball is placed on top of nonwoven textile with some orientation of fibres and after start of simulation process infiltrate inside, then when we change angle of wetting = dropping ball interpenetrate (0°) or dropping ball doesn't penetrate (90°).

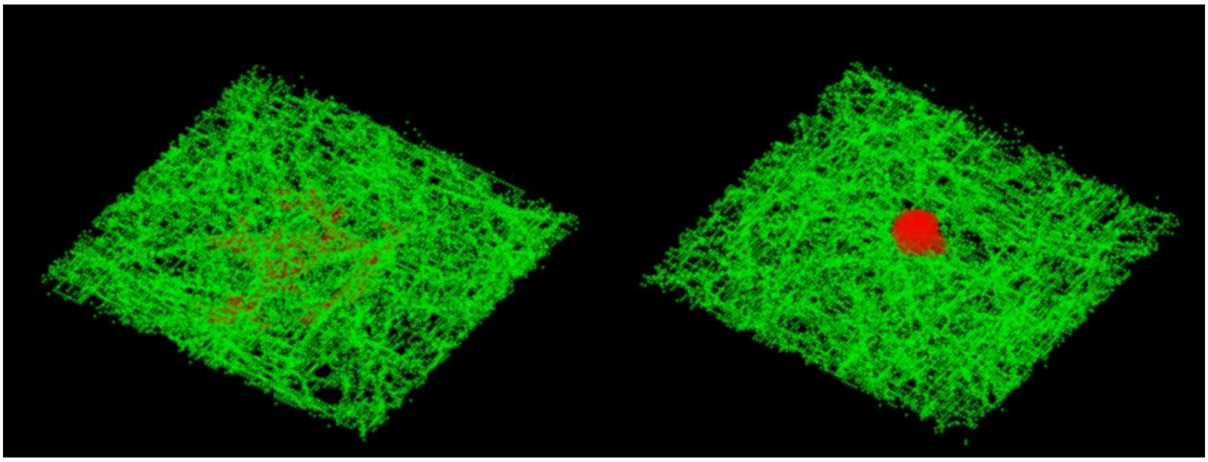

Figure 4. The result images present equilibrium state of liquid droplet versus fibrous nonwoven structure at the end of simulation process in two ultimate states of the system, liquid with high contact angle (left) and or liquid with low contact angle (right) in contact with randomly oriented fibrous material.

Interface

Occupied elements of 3D model imported in layers into as vertices. Then is apply volume effect on them (various color depending on fibre or liquid fluid element). Further is possible render or animate structures made by fibres with liquid interaction or even cut samples in desired positions with orthographic camera point of view. It works properly actually for very large data sets.

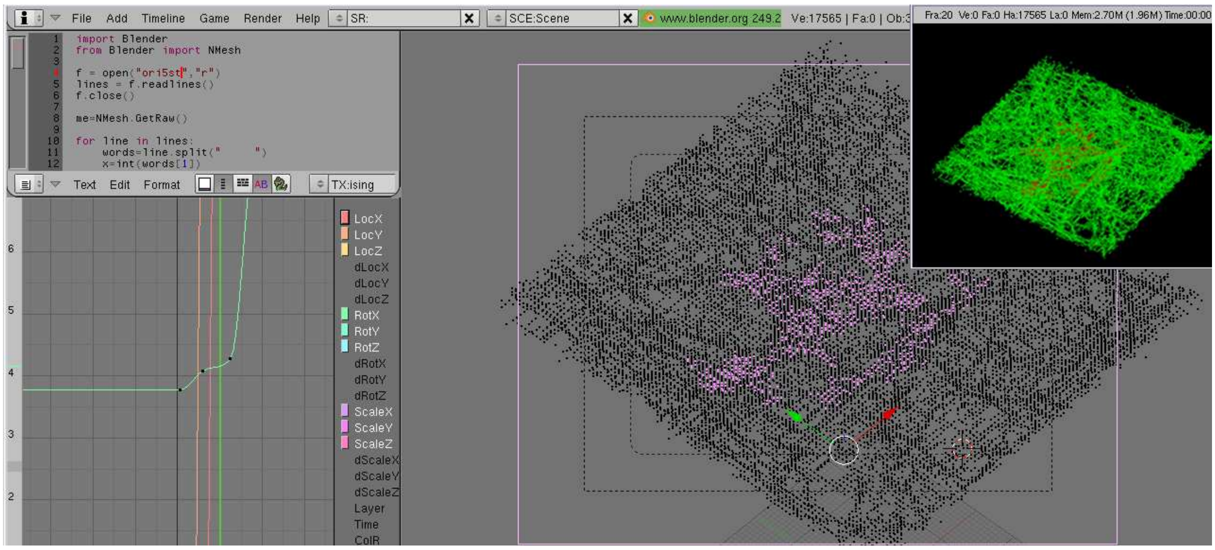

Figure 5. System of fibrous nonwoven material in computer workspace. Rendered image or linear sequence of images (right up).

Eventually is possible to use textured slices in a voxel visualization manner, like a 3D virtual reconstruction of human body from cuts obtained by medicine computer tomography devices.

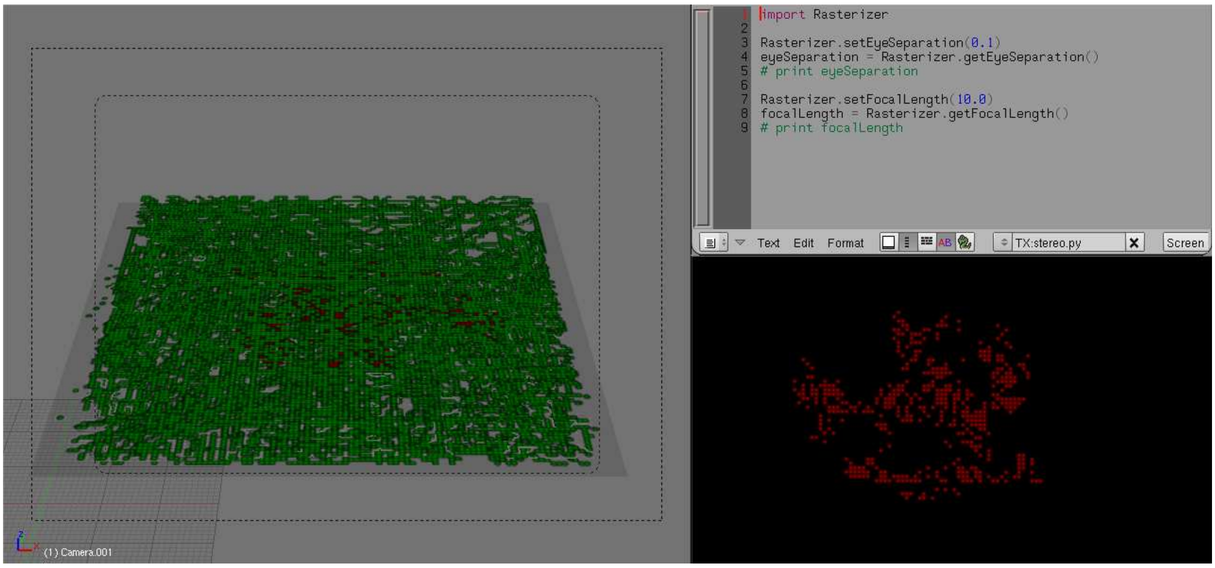

Figure 6. Reconstructed voxel slices (left) of fibrous nonwoven material. Textured image slice of droplet with alpha channel (right down).

Visualization

Furthermore it is also possible to present linear or even realtime content in low cost anaglyph stereoscopy or active virtual reality projection due much better immersion.

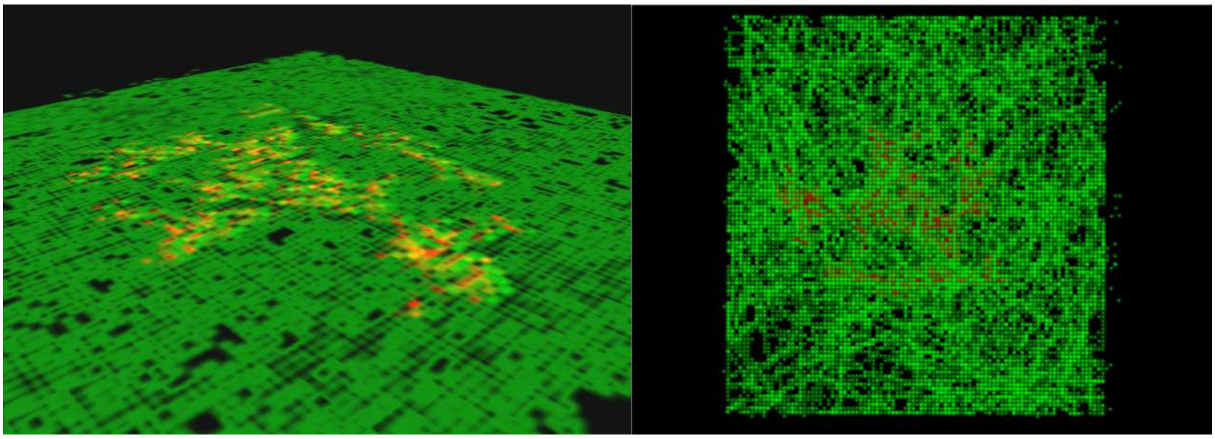

Figure 7. Perspective anaglyph of fibrous nonwoven material (left). Top view of complete fibrous system with an alpha channel slice (right).

Try out possibilities of scientific computing and visualisation in one's into realtime interactive game engine environment in a manner of supported realtime shaders as now GLSL.

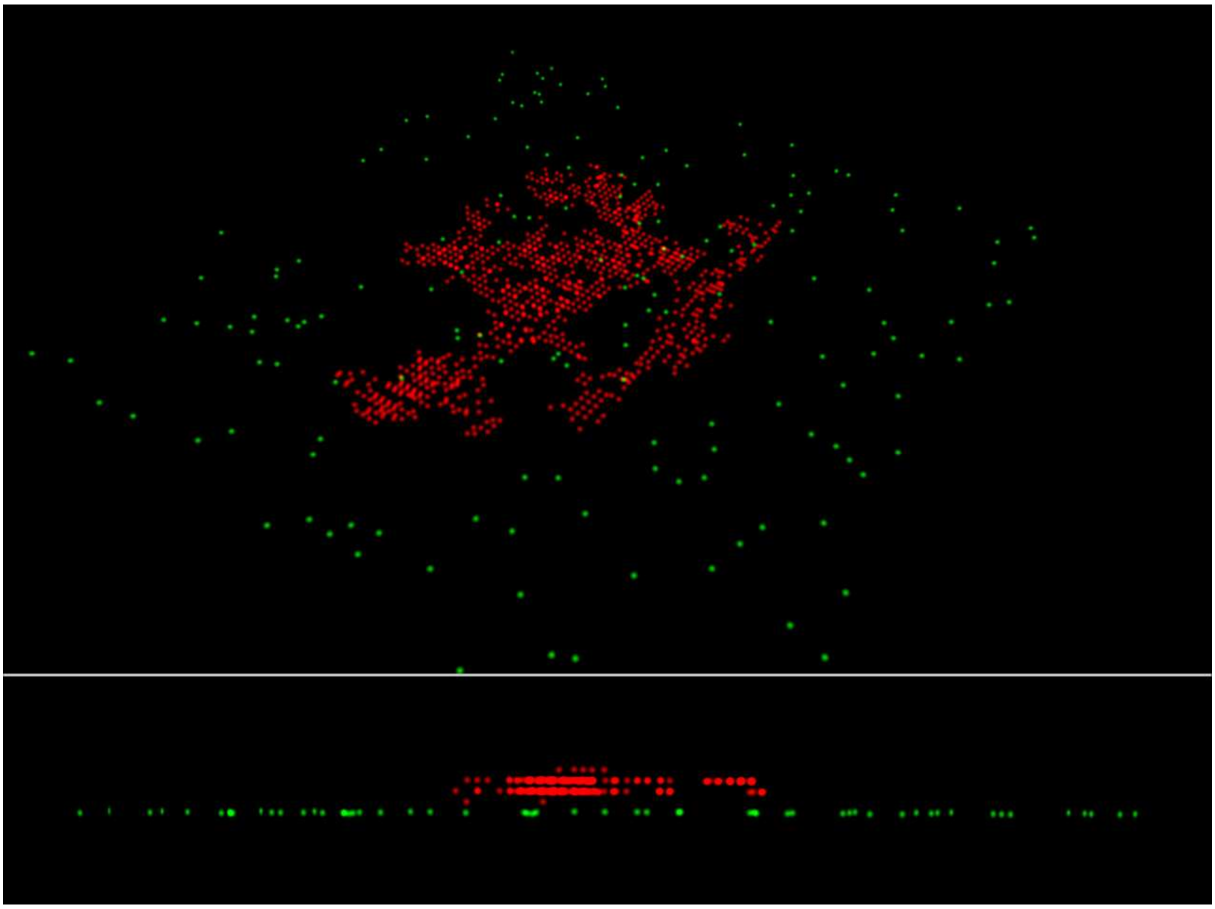

Figure 8. Realtime interactive visualization via GPU. Perspective camera view (top) and side view of fibrous system with droplets (down).

Parallel computing architecture is a programming approach for the performing scientific calculations on GPU as a data parallel computing device.

```
import GameLogic
cont = GameLogic.getCurrentController()
obj = cont.getOwner()

FragmentShader = """
	uniform sampler2D color;
	varying vec3 light_vec;
	varying vec3 normal_vec;
	void main() {
		vec3 l = normalize(light_vec);
		vec3 n = normalize(normal_vec);
		float ndotl = dot(n,l);
		gl_FragColor =  texture2D(color, gl_TexCoord[0].st)*ndotl;
	}
	"""

mesh_index = 0
mesh = obj.getMesh(mesh_index)
shader = mat.getShader()
shader.setSource( FragmentShader,1)
shader.setSampler('colorMap',0)
shader.setUniform1f('timer',(obj.timer))
```

Code 1. A piece of code in integrated interpreter for apply realtime pixelshader visualization via GPU.

Programming interface allows to implement algorithms using extensions to standard Python language used inside Blender [1].

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