MODELING OF A COLLECTION OF TENSEGRITY PARTICLES WITH A NON SMOOTH DISCRETE ELEMENT METHOD

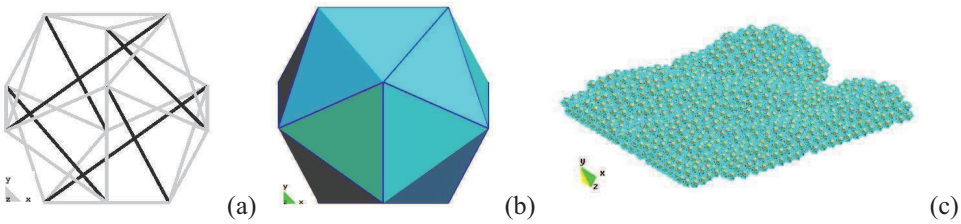
***E. Postek*[1], *F. Dubois*[2] *and R. Mozul*[2]**
[1]*Institute of Fundamental Technological Research, Warsaw, Poland*
[2]*Université de Montpellier 2, Montpellier, France*

1. Introduction

It is believed that the mechanical environment that cells experience is very important to their behaviour. A change of stresses in a cancer cell can cause that it starts to behave more like a healthy one [1].
A biological tissue made of a collection of cells can be modeled as a discrete system similar to a granular media. Since each cell is deformable and prestressed, we propose a dedicated DEM- FEM model of granular medium in which each particle is modeled through a tensegrity structure.

2. Tensegrity model of a cell

Since we aim to model a piece of tissue of a range of one million cells, we employ the simplest possible model for the cell. This is the icosahedron based tensegrity structure consisting of tendons (fair) and struts (dark) at first instance, Fig. 1 (a). The model enriched with membranes is shown in the Fig. 1 (b). The example of group of cells is shown in Fig. 1 (c).



(a) (b) (c)

Fig. 1. Single cell (a), cell with mebranes (b), group of cells (c)

3. Multibody approach

The vehicle for the model is the LMGC90 software [2], [3] in which we use the tensegrity model of the cell which, in fact, is a deformable viscoelastic particles model. In this approach, we simultaneously have to compute the contact between the particles and the stresses in the particles at each time instance.
Dynamics is written using the framework proposed by Moreau and Jean (see [3] for details). The set of equations of motion including the initial and the boundary conditions is of the form :

$$\mathbf{M}(\dot{\mathbf{q}}_{i+1} - \dot{\mathbf{q}}_i) = \int_{t_i}^{t_{i+1}} (\mathbf{F}(\mathbf{q}, \dot{\mathbf{q}}, s) + \mathbf{P}(s))ds + \mathbf{p}_{i+1} \tag{1}$$

$$\mathbf{q}_{i+1} = \mathbf{q}_i + \int_{t_i}^{t_{i+1}} \dot{\mathbf{q}} ds \tag{2}$$

where $\mathbf{M}$ is the mass matrix, $\mathbf{q}$ is the vector of generalized displacements, $\mathbf{P}(t)$ is the vector of external forces, $\mathbf{F}(\mathbf{q}, \dot{\mathbf{q}}, t)$ is the vector of internal forces including the inertia terms and $\mathbf{p}_{i+1}$ is the vector of impulse resulting from contacts over the time step.

While applying a Newton-Raphson procedure to the previous nonlinear system, which was integrated through a θ scheme, leads to the following equation which will be used in the NSCD method:

$$\tilde{\mathbf{M}}^k \Delta\dot{\mathbf{q}}_i^{k+1} = \mathbf{p}_{free}^k + \mathbf{p}_{i+1}^{k+1} \tag{3}$$

The effective mass matrix $\tilde{\mathbf{M}}^k$ writes as follows

$$\tilde{\mathbf{M}}^k = \mathbf{M} + h^2\theta^2\mathbf{K}^k \tag{4}$$

where h is the time increment, θ is the integration coefficient $[0.5, 1]$ and $\mathbf{K}$ is the tangent stiffness. The θ coefficient is usually taken as 0.5 yielding the Crank-Nicholson integration rule. The effective impulse vector of forces free of contact is of the form

$$\mathbf{p}_{free}^k = \tilde{\mathbf{M}}^k\dot{\mathbf{q}}_{i+1}^k + \mathbf{M}(\dot{\mathbf{q}}_i - \dot{\mathbf{q}}_{i+1}^k) + h[(1-\theta)(\mathbf{F}_i + \mathbf{P}_i) + \theta(\mathbf{F}_{i+1}^k + \mathbf{P}_{i+1})] \tag{5}$$

Contact impulses are computed using the NSCD method implemented in the LMGC90 software. First it will perform contacts detection between cells. Then the previous dynamics equations will be expressed in term of contacts unknowns (gap or relative velocity and contact impulse). Afterward a Non Linear Gauss-Seidel method computes the contacts impulses. Finally, the resulting impulse on cells nodes due to contacts impulses are added to the dynamics equation to compute the new velocities and positions.
Eventually a parallel version of the NSCD method can be used [2].

4. Concluding remarks

The presented scheme, based on a coupling of LMGC90 software and a dedicated modeling of cells, has been joined to an agent model able to take into account the effect of the stress evolution in the growing tissue [4]. The agent modeling is based on the FLAME framework (Flexible Large-scale Agent Modelling Environment) [5].

5. References

[1] C. Ainsworth (2008), Stretching the imagination, *Nature*, **456**, 696-699.

[2] M. Renouf, F. Dubois and P. Alart (2004). A parallel version of the Non Smooth Contact Dynamics Algorithm applied to the simulation of granular media *J. Comput. Appl. Math.*, **168**, 375-382.

[3] F. Radjai, F. Dubois (2011), Discrete-element Modelling of Granular Materials, *Wiley & Sons, New York*.

[4] E. Postek (2012), Concept of an Agent-stress Model of a Tissue, *accepted in Techn. Mechanik*.

[5] S. Adra, T. Sun, S. McNeil, M. Holcombe, R. Smallwood (2010), Development of a three dimensional multiscale computational model of the human epidermis, *PLoS ONE*, **5**, 1-13.