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MODELLING OF A COLLECTION OF NON-RIGID PARTICLES WITH SMOOTH DISCRETE ELEMENT METHOD

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1. Introduction

Usually, the models of generation of the cell colonies use the quasi-static discrete element approach to evaluate the contact forces between the cells [1]. The forces are necessary for evaluation of the mechanotransduction phenomena [2]. In contrast to this approach we use compliant particles. The use of the non-rigid particles changes the stresses distribution in the particles assembly. Even intuitively, it is closer to reality.

2. Cell colony

The cell colony stands for a piece of tissue. We employ a non-rigid model of a single particle of equivalent stiffness to the cell. The calibration is done following the paper [3].

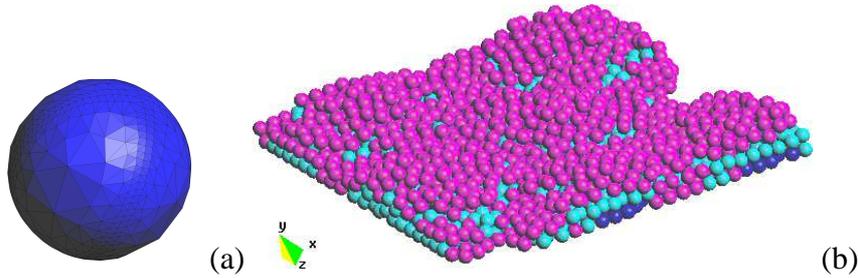(a)   (b)
Fig. 1. Single cell (a) Group of cells (b).

The group of cell avatars in Fig. 1 (b) has been generated employing the agent model in the framework of the FLAME platform (Flexible Large-scale Agent Modelling Environment) [1]. It consists of the stem cells, the TA cells and the Committed cells. The avatars are replaced with the equivalent stiffness cells, Fig. 1 (a).

3. Multibody approach

We apply the program LMGC90 [4], [5] with the possibility of modelling of contact of large number of compliant particles that are discretized with finite elements.

The governing equations are written in the framework of the approach that was proposed by Moreau and Jean [4]. The set of equations of motion including the initial and the boundary conditions takes the form:

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

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.

The integration with the θ scheme of the above system of equations leads to the equation:

$$(2) \qquad \tilde{\mathbf{M}}^k \Delta \dot{\mathbf{q}}_i^{k+1} = \mathbf{p}_{free}^k + \mathbf{p}_{i+1}^{k+1}$$

The effective mass matrix $\tilde{\mathbf{M}}^k$ reads:

$$(3) \qquad \tilde{\mathbf{M}}^k = \mathbf{M} + h^2 \theta^2 \mathbf{K}^k$$

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 taken as 1.0 yielding the Newton-Raphson integration rule. The effective vector of forces free of contact is of the form:

$$(4) \qquad \mathbf{p}_{free}^k = \tilde{\mathbf{M}}^k \dot{\mathbf{q}}_{i+1}^k + \mathbf{M}(\dot{\mathbf{q}}_i - \dot{\mathbf{q}}_{i+1}^k) + h[(1-\theta)(\mathbf{F}_i + \mathbf{P}_i) + \theta(\mathbf{F}_{i+1}^k + \mathbf{P}_{i+1})]$$

Contact impulses are computed using the NSCD method implemented in the LMGC90 software platform. Firstly, it will perform contacts detection between cells. Then the previous dynamics equations will be expressed in term of contact 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. We use the Open-MPI parallel version of the program [2].

4. Concluding remarks

With the presented scheme we calculate contact forces between the particles. The scheme that is based on a coupling of LMGC90 software and the 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 [6].

5. References

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