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Parallel Version of a Design Sensitivity Tensegrity Code

Introduction

The cytoskeleton is a tensegrity structure (1). The mechanics is important to the cells: *''Change the mechanical stresses on cancer cells and they can start to behave more like healthy ones''* (2). The displacements and stresses change in the biological materials due to the growth, division and death of the cells (3). The cells receive signals for the actions. This constitutes the agent-stress based models of the tissue (4).

Methodology

The cell consists of nucleus, actins, microtubules, membranes and collagen, Fig. 1.

The actins and microtubules are tendons and struts. They are viscoelastic, prestressed, keep volume when deformed, stiffen when tensioned. The icosahedral tensegrity structure is in Fig. 2.

The data is in (3). We perform the design sensitivity analysis, DSA (5). The fields are sensitive to the lengths of the elements. The parameters are grouped into clusters - the cells and the groups of clusters. This is the mechanotransduction sensitivity.

Formulation

We adopt the Updated Lagrangian formulation,

$$(1)\quad \left(\left(\int_{\Omega^t} \mathbf{B}_L'^T\, {}_t^t\bar{\tau}\mathbf{B}_L'\, d\Omega^t\right) + \int_{\Omega^t} \mathbf{B}_L^T \Delta\mathbf{S}\, d\Omega^t\right)\Delta\mathbf{q} = \int_{\Omega^t} \mathbf{N}^T\Delta\mathbf{f}\, d\Omega^t + \int_{\partial\Omega_\sigma^t} \mathbf{N}^T\Delta\mathbf{t}\, d\left(\partial\Omega_\sigma^t\right)$$

where $\mathbf{B}_L'^T$ and $\mathbf{B}_L^T$ are the nonlinear and linear operators, $\mathbf{N}$ is the shape functions matrix, $\Delta\mathbf{S}$ is the stress increment, $\bar{\tau}$ is the Cauchy stress matrix, $\Delta\mathbf{q}$ is the displacement increment, $\Delta\mathbf{f}$ and $\Delta\mathbf{t}$ are the body forces and the boundary tractions.

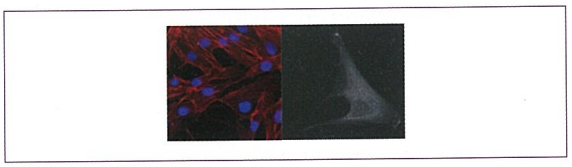

Fig. 1. – Fibroplasts; a) cells with nuclei b) cross-section with enhanced actins (credit: Dr Louise Smith).

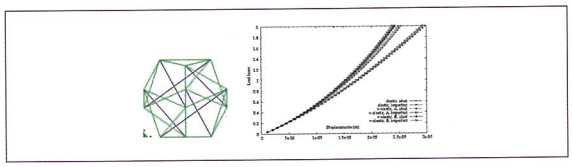

Fig. 2. – Cell a) compressed struts – blue, tensioned tendons – yellow b) stiffening.

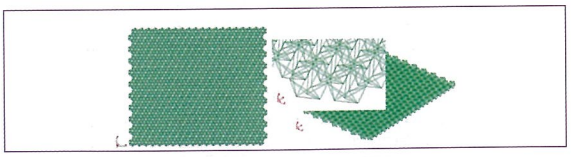

Fig. 3. – 400 cells.

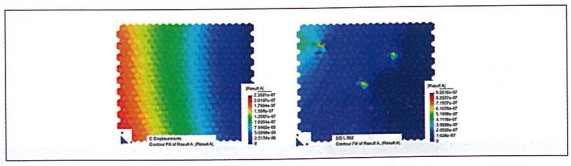

Fig. 4. – Process: a) scratch appears b) finishes.

The $\Delta\mathbf{S}$ depends on total stress $\mathbf{S}$, shear modulus (G), bulk modulus (K) and strain $\Delta\mathbf{E}$,

$$(2)\quad \Delta\mathbf{S} = \mathbf{D}^{const}(\mathbf{S}, G, K)\Delta\mathbf{E} \quad G(t) = G_o + \sum_{i=1}^{n} G_i \exp\left(\frac{-t}{\lambda_i}\right)$$

t is time and λ_i are the relaxation times of the parallel dampers.

The differentiated equation (1) w.r.t. the design variable h is of the form

$$(3)\quad \left(\left(\int_{\Omega^t} \mathbf{B}_L'^T\, {}_t^t\bar{\tau}\mathbf{B}_L'\, d\Omega^t\right)\frac{d\Delta\mathbf{q}}{dh} + \int_{\Omega^t} \mathbf{B}_L^T\mathbf{S}\, d\Omega^t\right) = \frac{d\Delta\mathbf{Q}}{dh} - \frac{d\Delta\mathbf{F}}{dh}\Big|_{\Delta\varepsilon \text{ fixed}}$$

$\Delta\mathbf{Q}$ is the *r.h.s.* of (1) and $\Delta\mathbf{F}$ is the internal forces increment

$$(4)\quad \frac{d\Delta\mathbf{F}}{dh} = \frac{d}{dh}\left(\left(\int_{\Omega^t} \mathbf{B}_L'^T\, {}_t^t\bar{\tau}\mathbf{B}_L'\, d\Omega^t\right) + \int_{\Omega^t} \mathbf{B}_L^T\Delta\mathbf{S}\, d\Omega^t\right)\Big|_{\Delta\varepsilon \text{ fixed}}$$

The (3) and (4) define the direct differentiation method.

Numerical aspects

The parallel program includes the solver MUMPS (6). We use the Newton-Raphson technique for solving the (1). The DSA creates r.h.s (4) to the (3). We solve as many equations as the design variables using last triangularized stiffness after the iteration loop.

Example

We analyze a honeycomb pattern of the single layer cell matrix, Fig 3. The layer slides and is fixed. It is tensioned on the left. The tissue is scratched after 0.1 sec. We observe the sensitivity fields of the displacements w.r.t. the design variables: 3 cells in which all microtubules change their lengths. The sensitivities are shown at the start and the end of the process, Fig. 4.

The most sensitive places are close to the chosen cells when the scratch appears. Finally, the gradients become distributed on left side of the scratch. The change of the design parameters in the cells affects entire structure and the gradients are of range higher. The structure approaches failure.

Remarks

We present the DSA parallel algorithm valid for nonlinear path dependent systems. The application is the computational systems biology.

References

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