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Multiscale modeling of the dynamics of multicellular systems[1]

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Describing the biomechanical properties of cellular systems, regarded as complex highly viscoelastic materials, is a difficult problem of great conceptual and practical value. Here we present a novel approach, referred to as the Cellular Particle Dynamics (CPD) method, for: (i) quantitatively relating biomechanical properties at the cell level to those at the multicellular and tissue level, and (ii) describing and predicting the time evolution of multicellular systems that undergo biomechanical relaxations. In CPD cells are modeled as an ensemble of cellular particles (CPs) that interact via short range contact interactions, characterized by an attractive (adhesive interaction) and a repulsive (excluded volume interaction) component. The time evolution of the spatial conformation of the multicellular system is determined by following the trajectories of all CPs through integration of their equations of motion. Cell and multicellular level biomechanical properties (e.g., viscosity, surface tension and shear modulus) are determined through the combined use of experiments and theory of continuum viscoelastic media. The same biomechanical properties are also "measured" computationally by employing the CPD method, the results being expressed in terms of CPD parameters. Once these parameters have been calibrated experimentally, the formalism provides a systematic framework to predict the time evolution of complex multicellular systems during shape-changing biomechanical transformations. By design, the CPD method is rather flexible and most suitable for multiscale modeling of multicellular system. The spatial level of detail of the system can be easily tuned by changing the number of CPs in a cell. Thus, CPD can be used equally well to describe both cell level processes (e.g., the adhesion of two cells) and tissue level processes (e.g., the formation of 3D constructs of millions of cells through bioprinting).

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