Exposé

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1 Introduction

Computational models of cell behavior can be useful to simulate and reiterate experiments. In addition, they can show us how well our understanding models reality. One popular model is the Cellular Potts Model (CPM), where each cell is modeled as a set of connected pixels or voxels on a two- or three-dimensional lattice. To simulate biological processes involving thousands of cells, large lattices are needed. Due to the local nature of the computations involved, the CPM lends itself well to distributed programming.

In order to be true to *in vivo*/*in vitro* findings, such *in silico* models must take into account a multitude of factors influencing cell behavior. One such factor is the Extracellular Matrix (ECM) that cells exist in. In this work we will focus on the viscoelasticity of the collagen networks in the ECM. We explore models of viscoelasticity that, similar to the CPM itself, employ local interactions to model global effects. In this manner the simulations remain parallelizable. Additionally, we investigate the performance of our model using different implementations on both CPUs and GPUs.

2 Research

2.1 The Cellular Potts Model (CPM)

The CPM [5] models cells as sets of sites on a square lattice which are usually connected. Each lattice site is assigned the integer cell ID of the cell it belongs to.

The behavior of the cells is regulated by the Hamiltonian H, which represents the energy of a particular lattice. The Hamiltonian consists of at least a term for the adhesion between cells on the lattice, but can be extended by other terms such as cell volume or alignment.

To advance the CPM, a Monte-Carlo Step (MCS) is performed: The cell ID of a random lattice site is changed to the cell ID of one of its neighbors and the difference in energy ΔH is calculated. The update is always accepted if the energy decreases. If the energy does not decrease, the update is accepted probabilistically, where greater increases are less probable. Repeated MCSs minimize H.

From an implementor's perspective, the CPM has a great advantage over other approaches to cell simulation such as agent-based modeling: Since updates happen on a square lattice and changes in energy can be calculated locally, it

lends itself well to distributed programming. Cells in Silico (CiS) [2] is a parallel implementation of the CPM based on the Neoteric Autonomous Stencil code for Jolly Algorithms (NAStJA) framework [1]. NAStJA offers an abstraction layer for implementing stencil codes on the Message Passing Interface (MPI), making it possible to leverage large-scale parallelism for CiS.

2.2 The Extracellular Matrix (ECM)

Sketch the ECM (2 sentences)

While the ECM consists of a variety of components [4], we focus on a single essential component: Fibrous collagen networks and their viscoelasticity. ECM viscoelasticity has been established as an important factor in cell behavior [3]. For example, the ECM confines cells and restricts processes such as migration, spreading, growth and mitosis. These processes also affect the ECM and can lead to permanent deformation. In turn, this deformation can have an influence on cell behavior, resulting in self-reinforcing effects (see for example [6]).

In the next section we list a few current approaches for modeling the ECM in the CPM.

2.3 Models of the ECM in the CPM

2.4 Models of Viscoelastic Materials

3 Contribution

3.1 Method

3.2 Challenges

Acronyms

CiS Cells in Silico. 2

CPM Cellular Potts Model. 1, 2

CPU Central Processing Unit. 1

ECM Extracellular Matrix. 1, 2

GPU Graphics Processing Unit. 1

MCS Monte-Carlo Step. 1

MPI Message Passing Interface. 2

NAStJA Neoteric Autonomous Stencil code for Jolly Algorithms. 2

References

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