1.1	**Proposal**	Master thesis project
1.2	**Name**	Hybrid Cellular Potts and Molecular Dynamics Modeling of Endothelial Monolayer Mechanics
1.3	**Description**	Endothelial cell (EC) monolayers form the inner lining of blood vessels and play a crucial role in maintaining vascular barrier integrity. The mechanical properties of the endothelium, including tensile strength, elasticity, and response to mechanical stress, are fundamental to proper barrier function and cardiovascular health. Disruption of endothelial mechanics contributes to various pathological conditions including atherosclerosis, inflammation, and barrier dysfunction. The endothelium exhibits complex mechanical behavior arising from the interplay between individual endothelial cells and their surrounding extracellular matrix (ECM). Understanding this mechanical reciprocity requires computational approaches that can capture both cellular dynamics and ECM mechanics at appropriate scales. **Objectives:** **• Hybrid Model Application and Extension** Adapt the existing hybrid Cellular Potts–Molecular Dynamics (CPM–MD) model[1, 2] to investigate the mechanical properties of endothelial monolayers. Depending on their interests and background, the student may either use and extend the available software to address the project's aims, or develop a new implementation based on the published modeling framework. **• Mechanobiological Analysis of EC Monolayers** Using the model, the student will simulate endothelial cells within the CPM framework interacting with an MD-modeled spring network representing the ECM, with the goal of characterizing how cell–ECM mechanical reciprocity governs the emergent tensile, elastic, and mechanical properties of the endothelial monolayer. **References:** [1] Erika Tsingos et al. "Hybrid cellular Potts and bead-spring modeling of cells in fibrous extracellular matrix". In: *Biophysical Journal* 122.13 (2023), pp. 2609–2622. [2] Koen AE Keijzer, Erika Tsingos, and Roeland MH Merks. "How cells align to structured collagen fibrils: A hybrid cellular Potts and molecular dynamics model with dynamic mechanosensitive focal adhesions". In: *Frontiers in Cell and Developmental Biology* 12 (2025), p. 1462277.
1.4	**Work environment**	The student will join a team of researchers from the Computational Science Lab (CSL) at the University of Amsterdam. This group includes experts in modeling of biological systems, with experience in CPM and MD framework. The student will be able to delve into the complexity of biological problems, contributing to a broader research focused on the role of RhoGTPases RhoA and RhoB in EC monolayer integrity.
1.5	**Expectations**	The student should have good programming skills (Python, C++) and previous experience with modeling of biological systems.
1.8	**Research Tags**	Computational Biology, Cellular Potts Model, Molecular Dynamics, Endothelial Cell Monolayer
1.9	**Programmes**	Computational Science (joint degree UvA/VU), Physics and Astronomy: Biophysics and Biophotonics (track–joint degree UvA/VU)
1.10	**Contact**	A. Acquaviva a.acquaviva@uva.nl